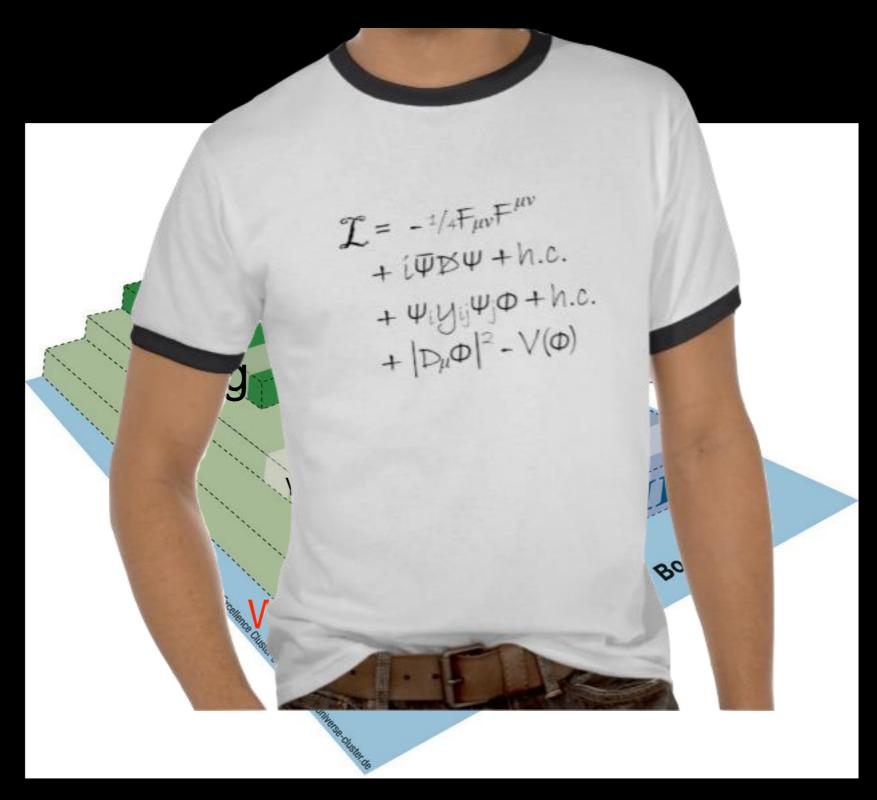
The RHIC & ATLAS Computing Facility Data Intensive Computing At The Scientific Frontier

Michael Ernst BNL Physics Department January 5, 2016

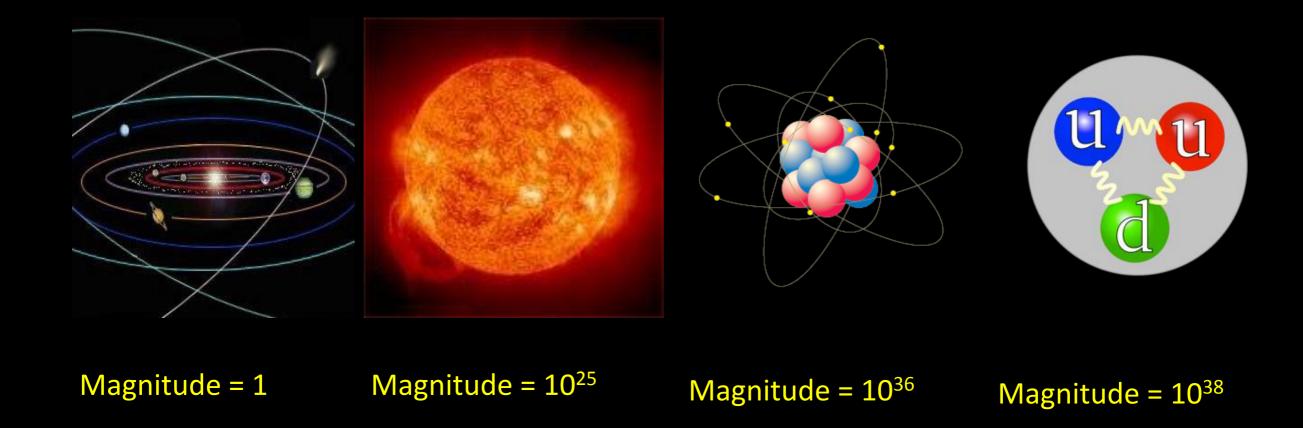
The Standard Model

A single, overarching theory that includes all types of matter in the Universe and explains how they interact...



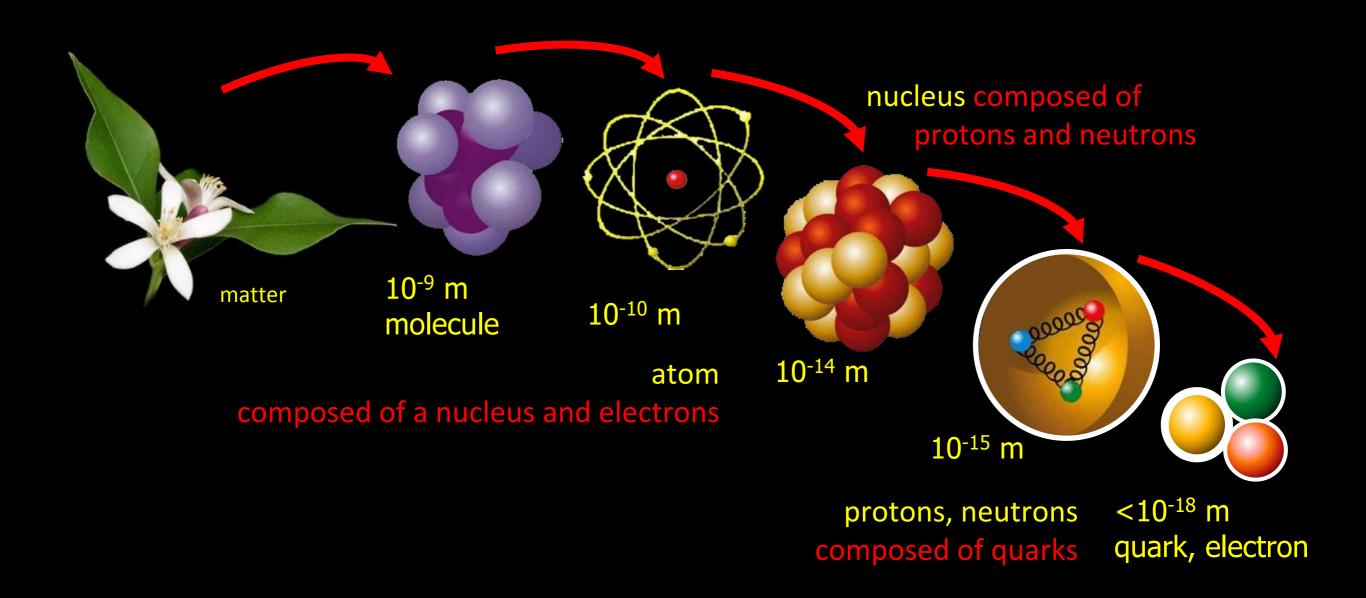
Must be self-consistent and explain all known physical observations!

The "Big Questions"



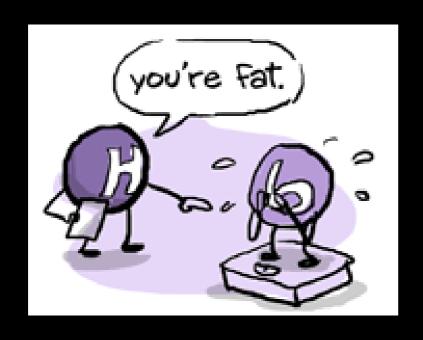
How does Gravity even fit in?

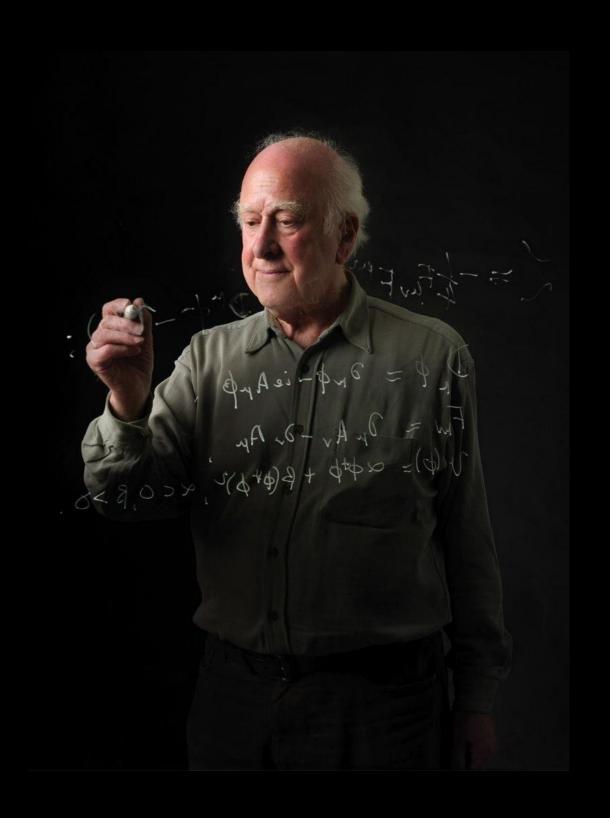
Where does this end?





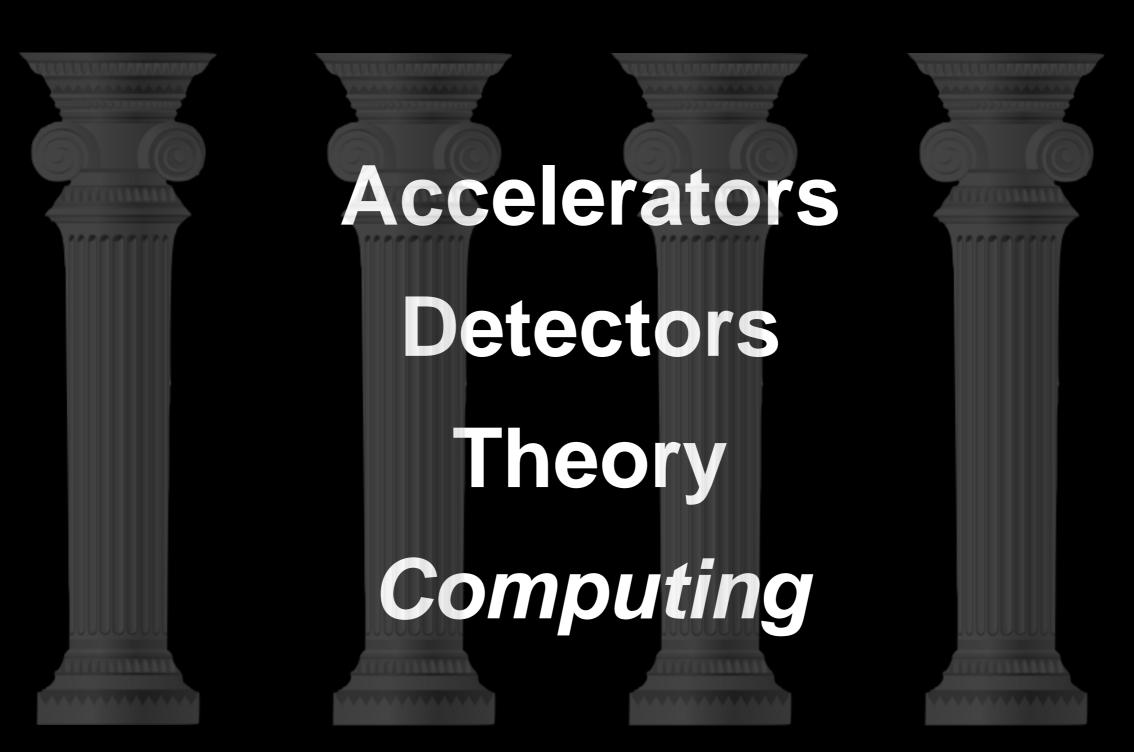
What is the nature of mass?

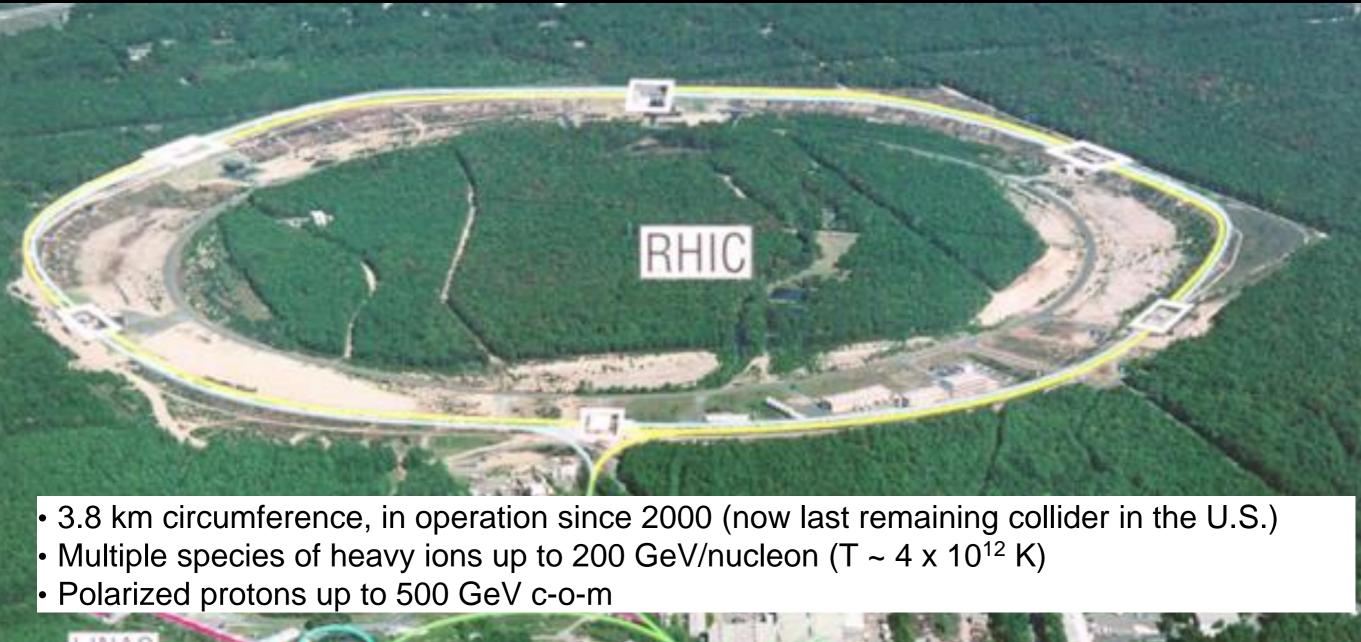




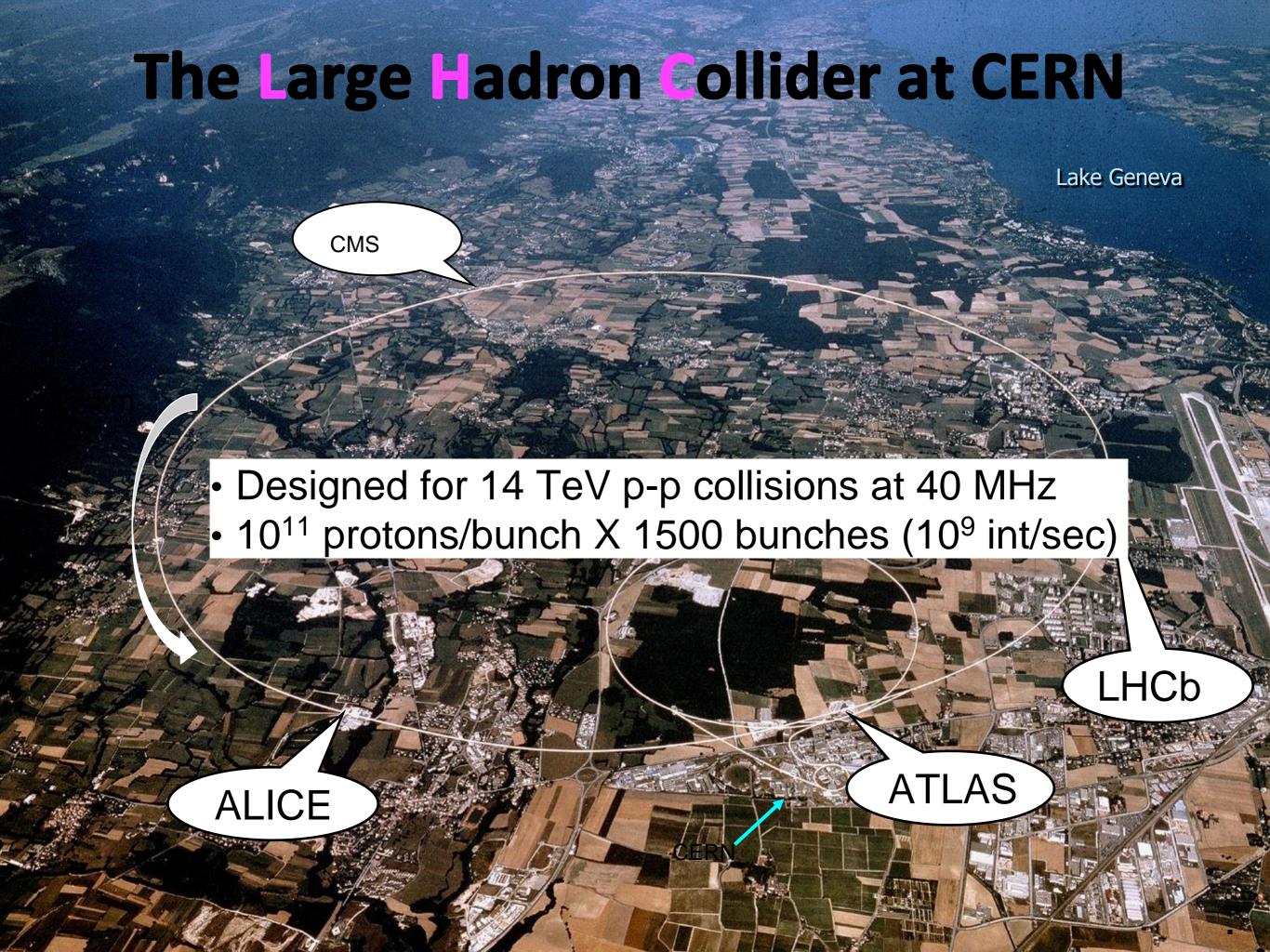
And what is the more fundamental underlying theory?

Four Pillars Of Modern Experimental Particle Physics Research

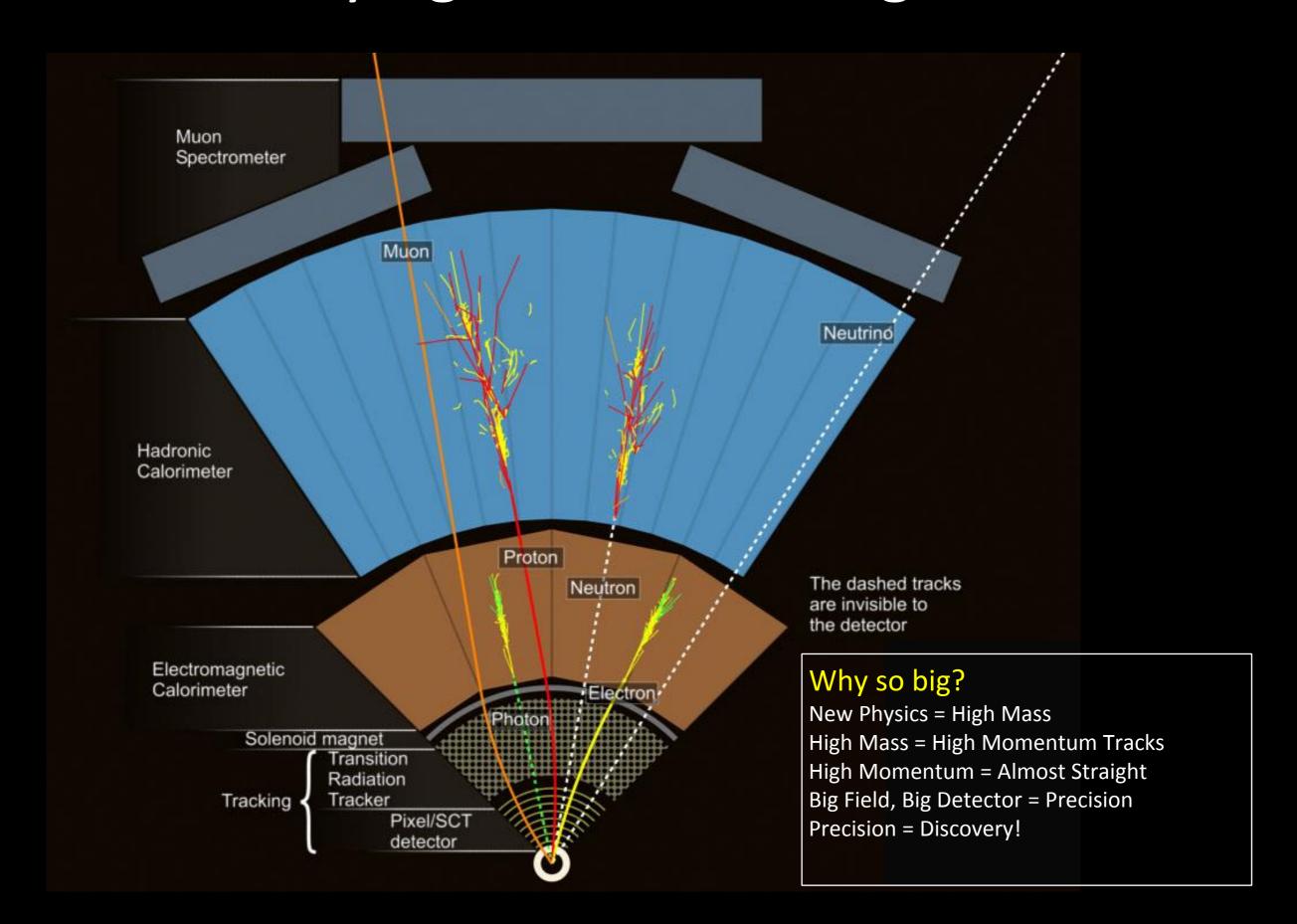




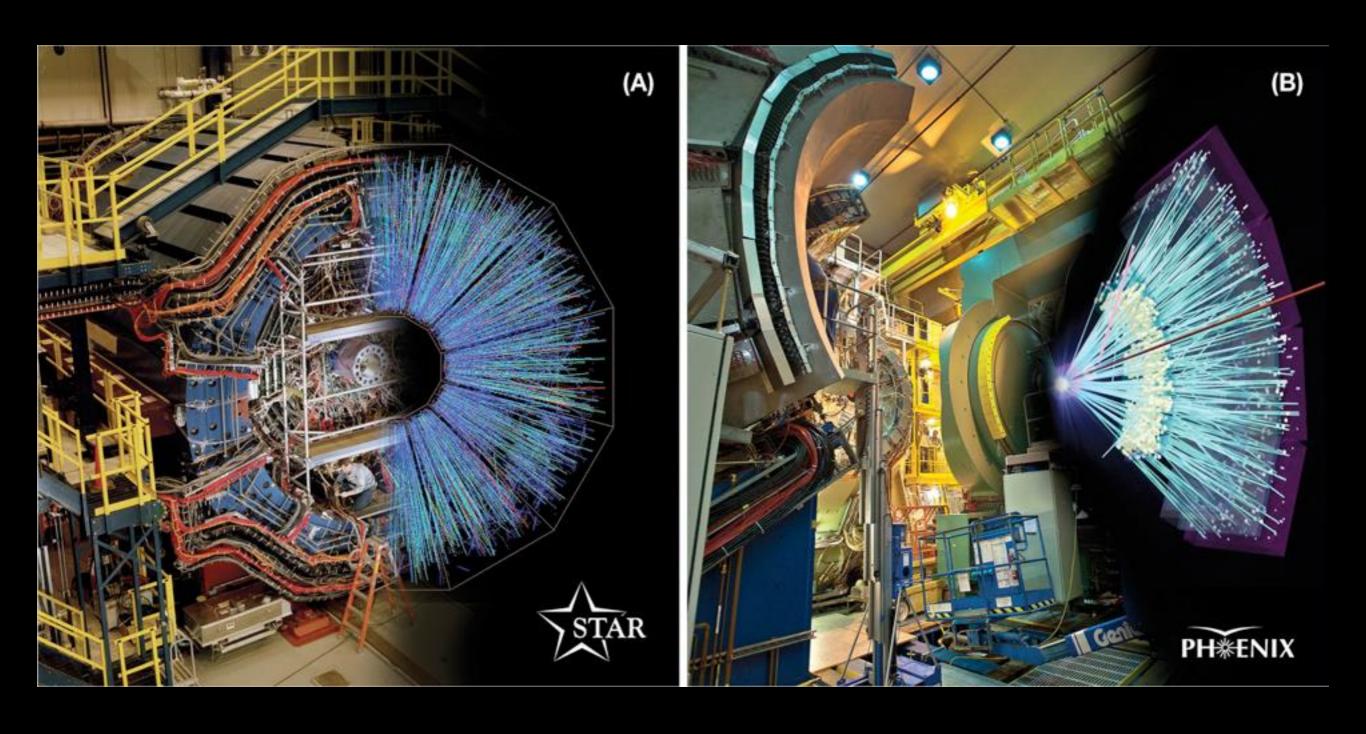




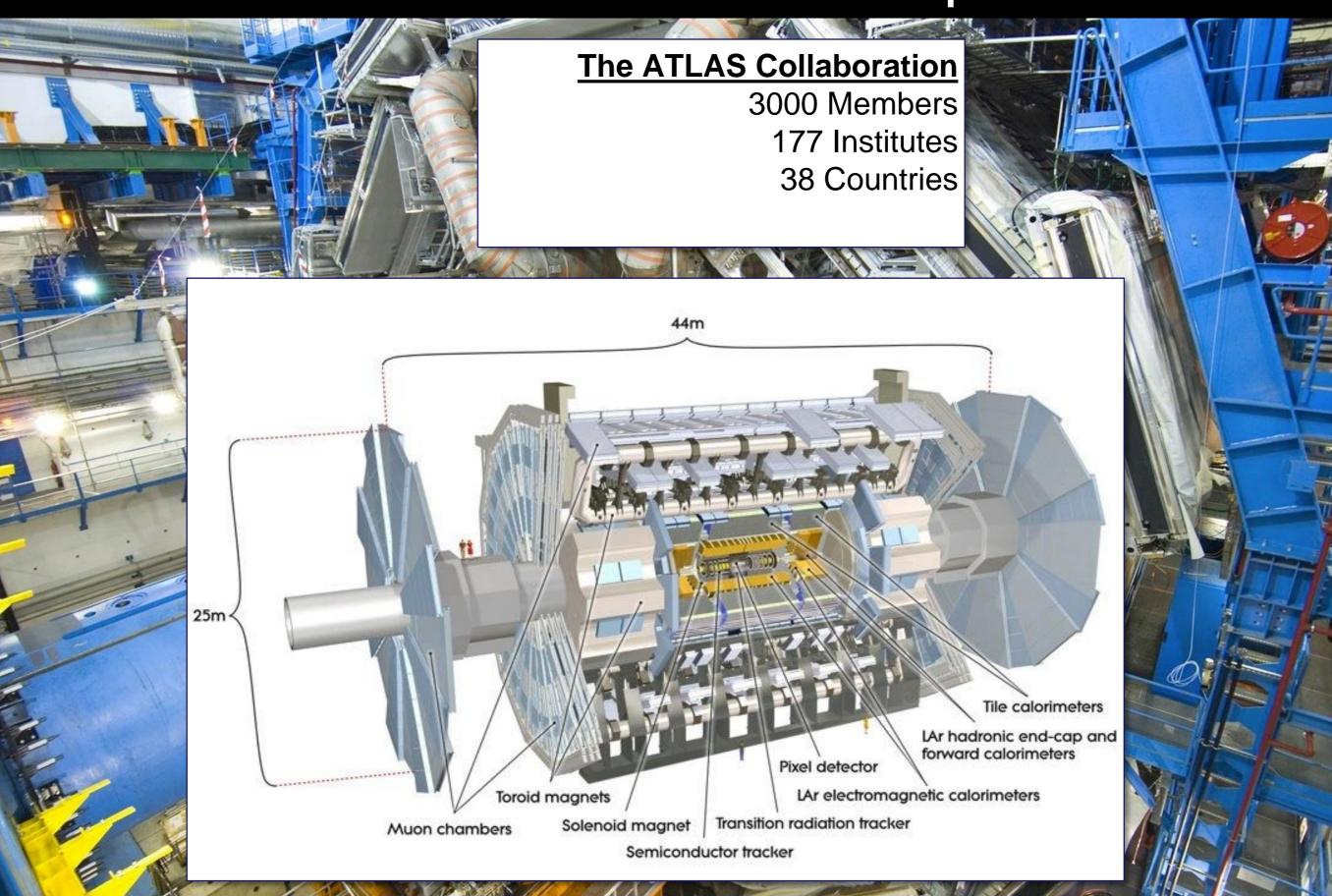
Identifying and Measuring Particle



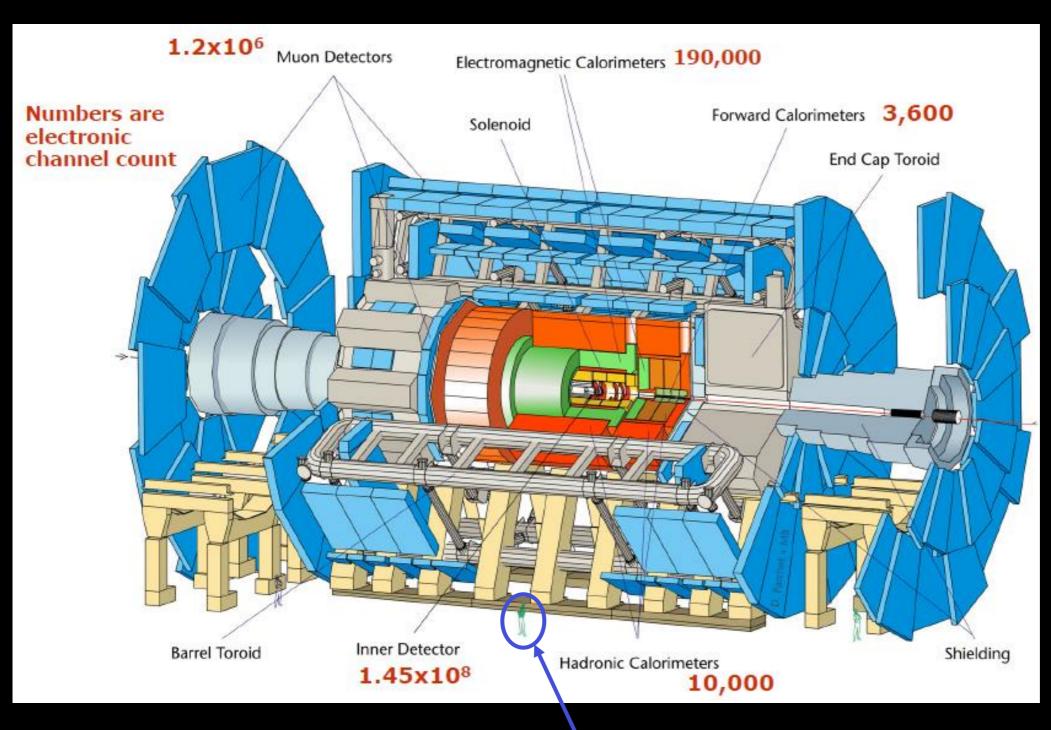
The RHIC Detectors



LHC Point 1: The ATLAS Experiment



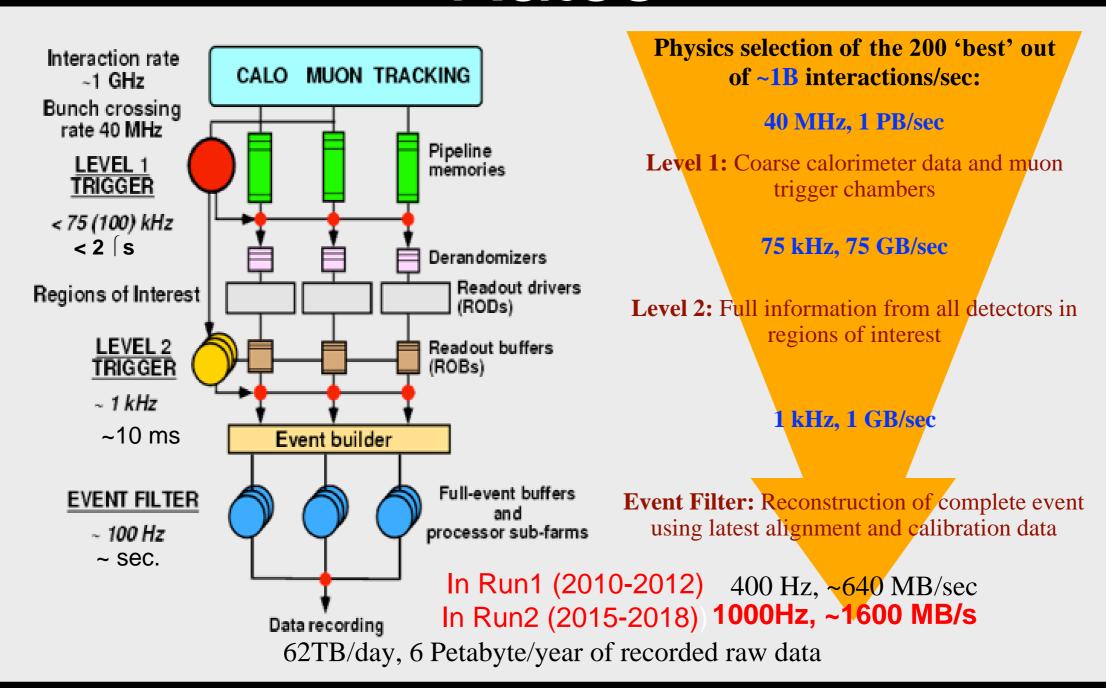
Electronic Channels At The ATLAS Detector



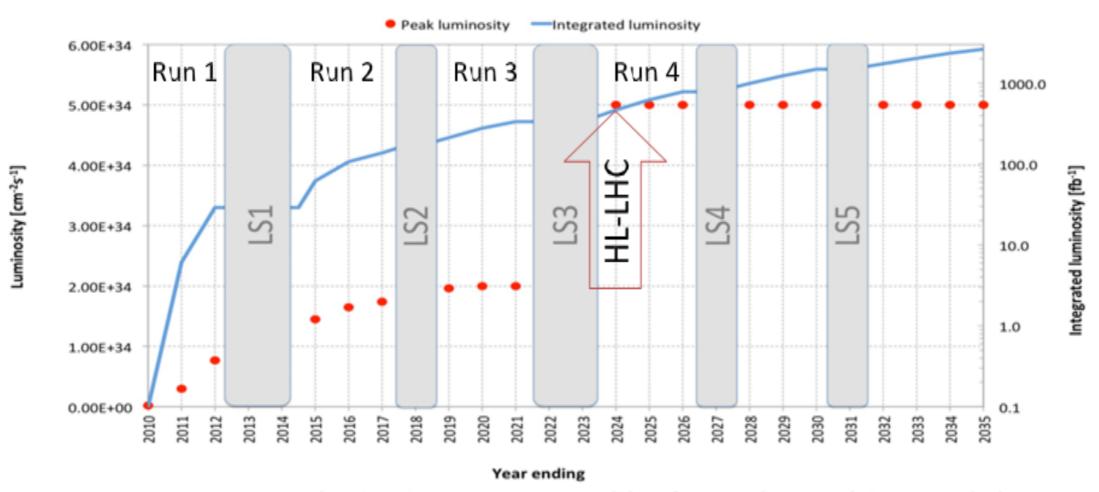
Length: ~ 46 m (150 ft) Radius: ~ 12 m (40 ft) Weight: ~ 7000 tons

~ 1800 miles of cables ~10 MW of electrical power

ATLAS Data Acquisition Rates



LHC Beyond Run 2 To the High Luminosity LHC (HL-LHC)



Trigger rates, event complexity increase steadily through machine and detector upgrades

~15 PB/year LHC raw data in Run 1; ~130 PB/year in 2021 (all 4 LHC Experiments)

Very rough estimate for new raw data per year in Run 4: 400 PB

Raw data is only the beginning, e.g. ATLAS dataset now is ~160 PB, ~50% on disk

Event complexity: pile-up reaches ~150 at HL-LHC (now ~30), multiplicity up 8x

Plenty of challenges ahead!

DAQ/HLT Upgrade Plans

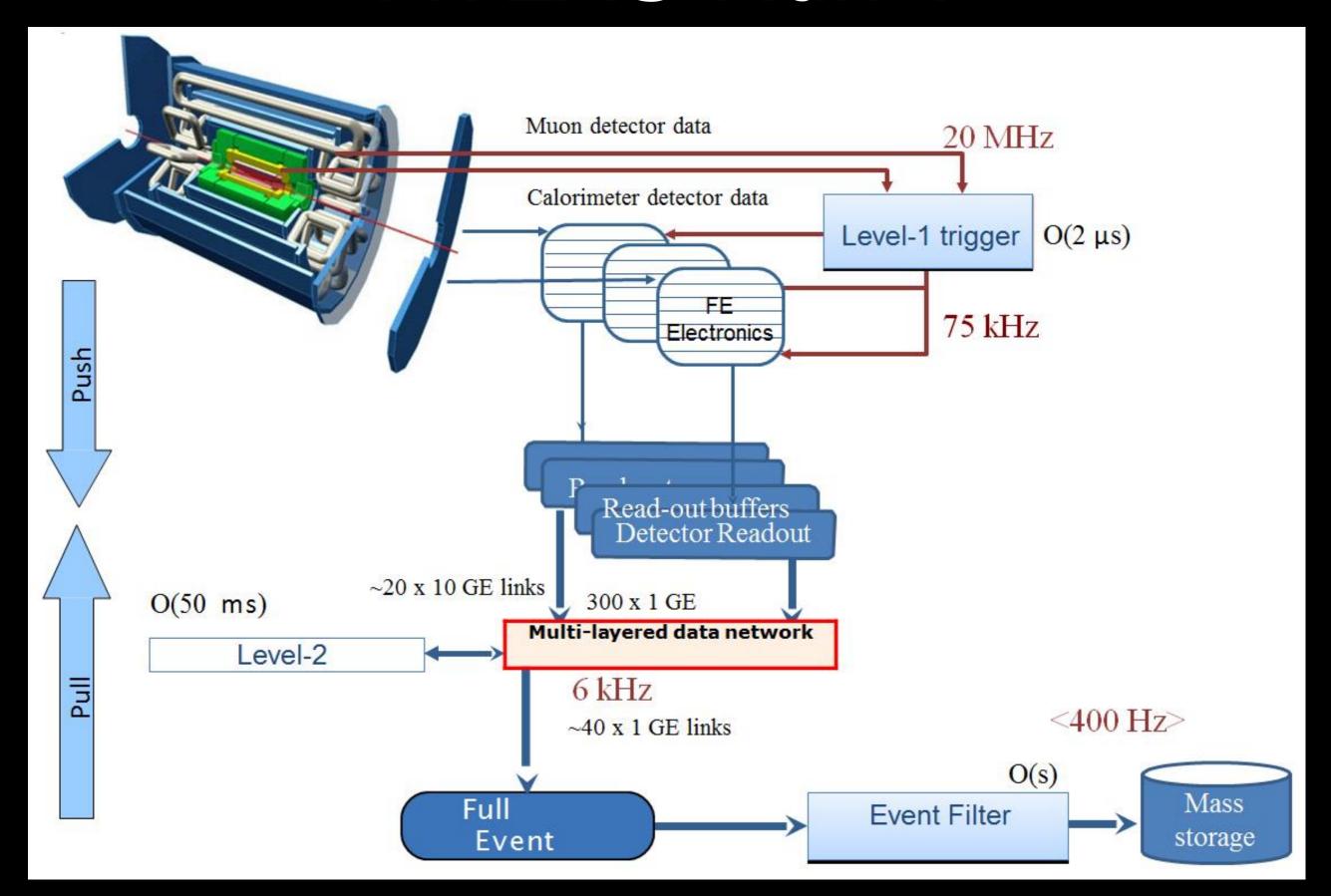
Driving Parameters

	# of Trigger levels	Leve	el-xRate (kHz)	Event Size (MB)	Network BW (GB/s)	Stor GB/s	age kHz
Run 1	3	Lvl-1 HLT	75 ~0.4	~1	10	0.5	~0.4
Run 2	2	Lvl-1 HLT	100 1	~2	50	1	1
Run 3	2	Lvl-1 HLT	100 1	~2	50	1	1
Run 4	3	Lvl-1 HLT	400 10	~5	2000	25	10

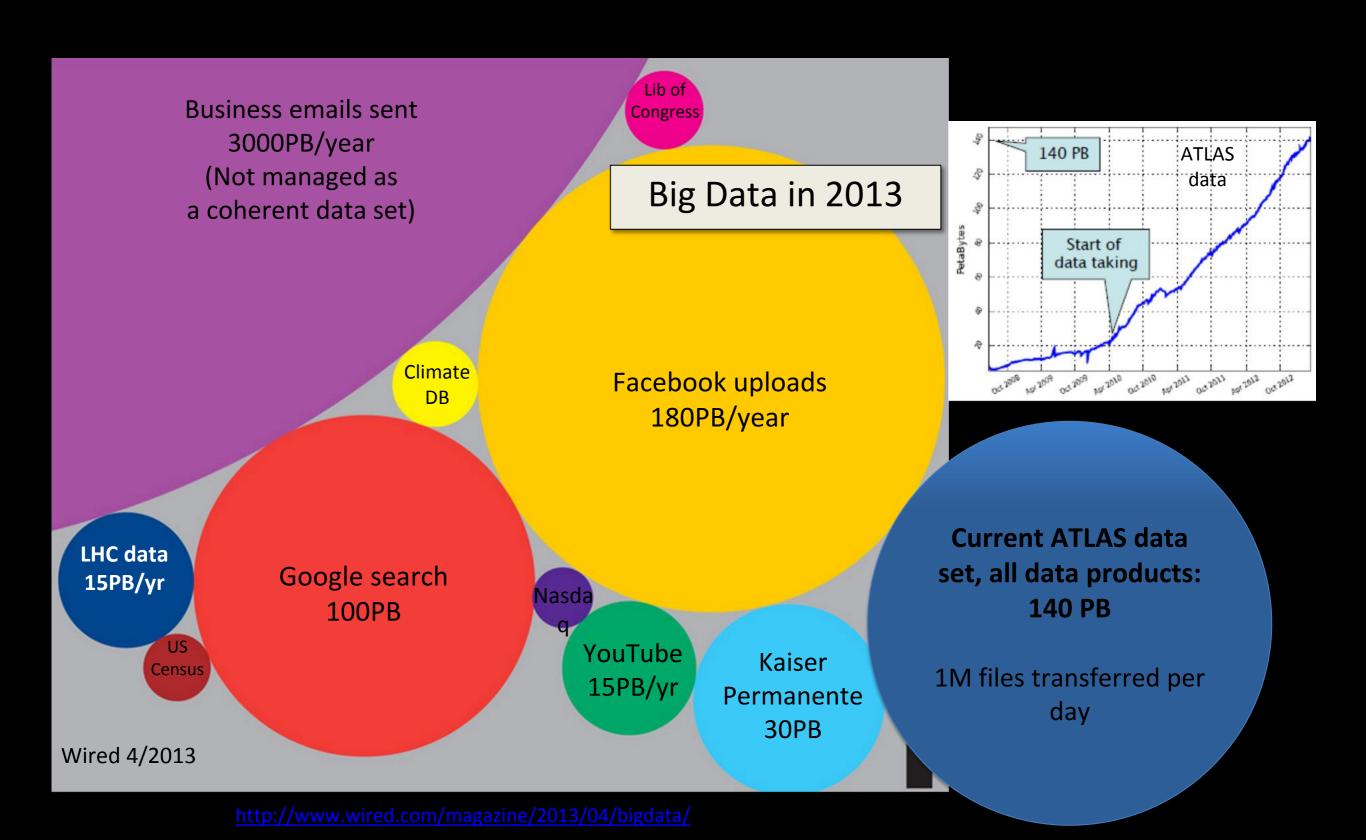
Notes

- Storage bandwidth includes compression factors
 Run 3: No major upgrades in the DAQ systems currently foreseen
- Run 4: Two stage hardware trigger (Level-0 and Level-1)

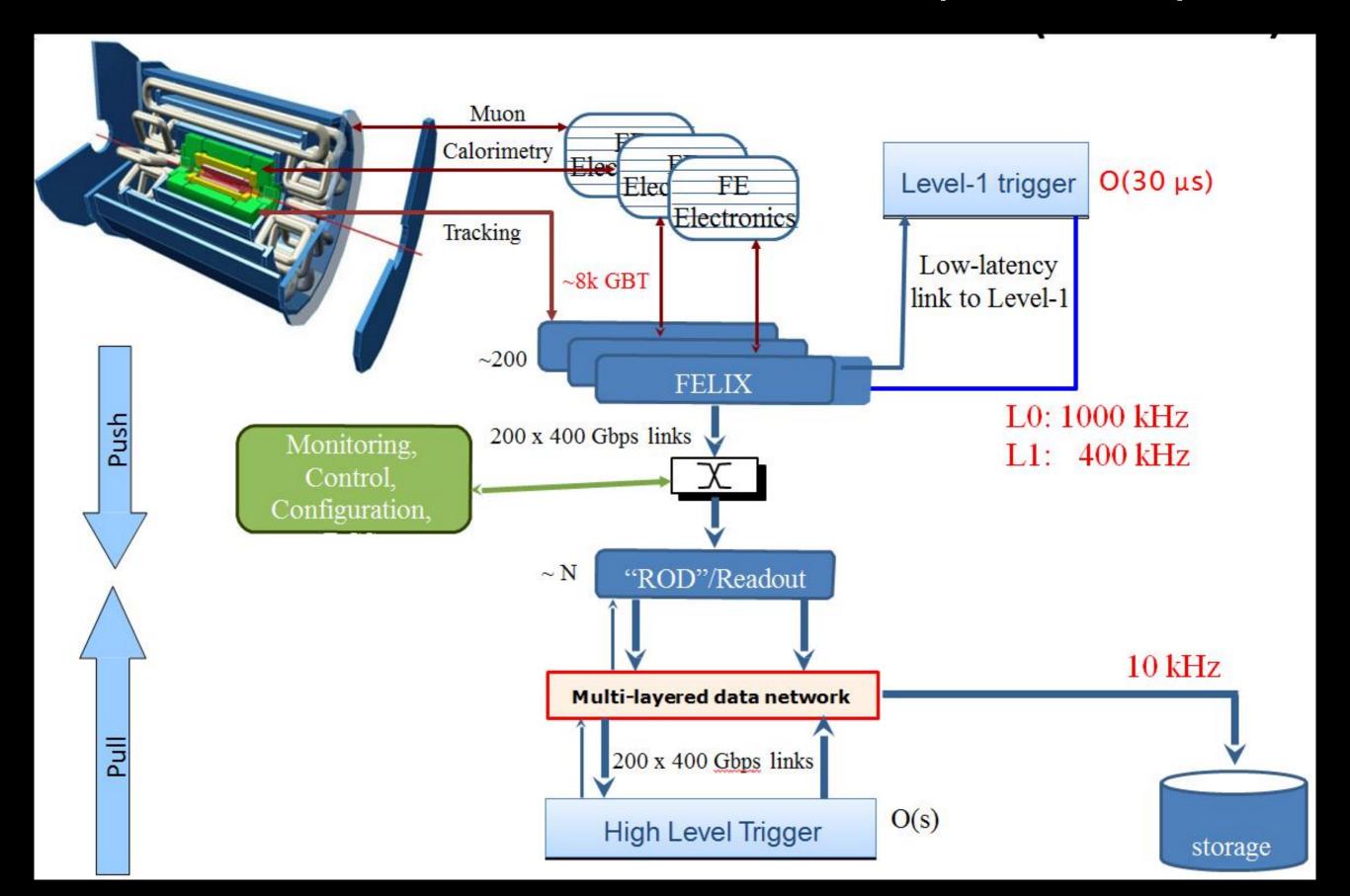
ATLAS Run 1



ATLAS is Big Data



Architecture in Run 4 (~2025)



Content Delivery Networks: Compare to Netflix

- HEP problem harder than Netflix?
 - Netflix delivers streaming video content to > 20M subscribers
 - Routinely quoted as the single largest user of bandwidth in the US
 - More than 30% of the traffic
- HEP has a different working point:
 - < # clients,
 - < distribution,
 - > bandwidth per client
- However, much larger data set
 - HEP can't make many multiple static copies
 - need different strategies instead:
 - make dynamic replicas and clean up when no longer useful
 - access data directly over the wide area networks

	NETFLIX	LHC Computing
Bandwidth per client	1.5Mbit/sec	1MByte/sec
Clients	1M*	200k cores
Serving	1.5Tbits	0.8Tbits
Total Data Distributed	12TB	140PB
Annual Budget	>\$4B	<\$.04B

Similar Problems: Not all files are equally accessed



e.g. Forward Physics ;-)

The Problem....

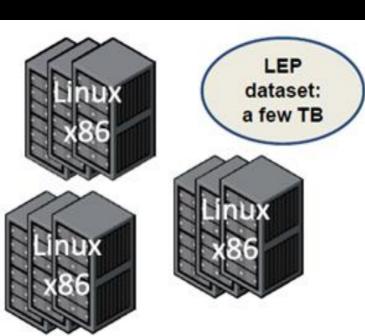


...the challenges of computing at the *Petabyte* scale

How to make a torrent of data available for science in the most efficient, transparent, and cost-effective way?



1980s: Plethora of architectures & OSes

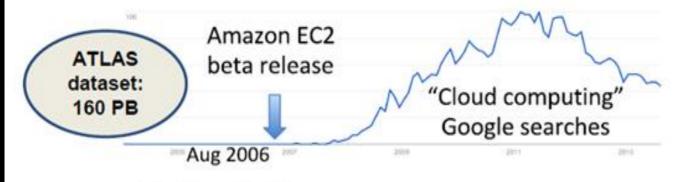


1990s: Uniform OS/architecture Linux/x86 standard for commodity cluster computing

HEP computing evolution – growing uniformity counters growing scale and complexity



2000s: Uniform fabric and access Globally federated resources enabled by network and grid

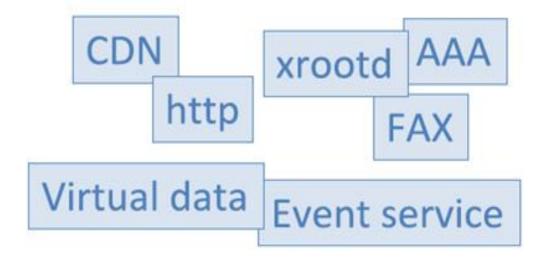


2010s: Uniform environment

VMs and clouds put the user in control

of the environment – take it with you

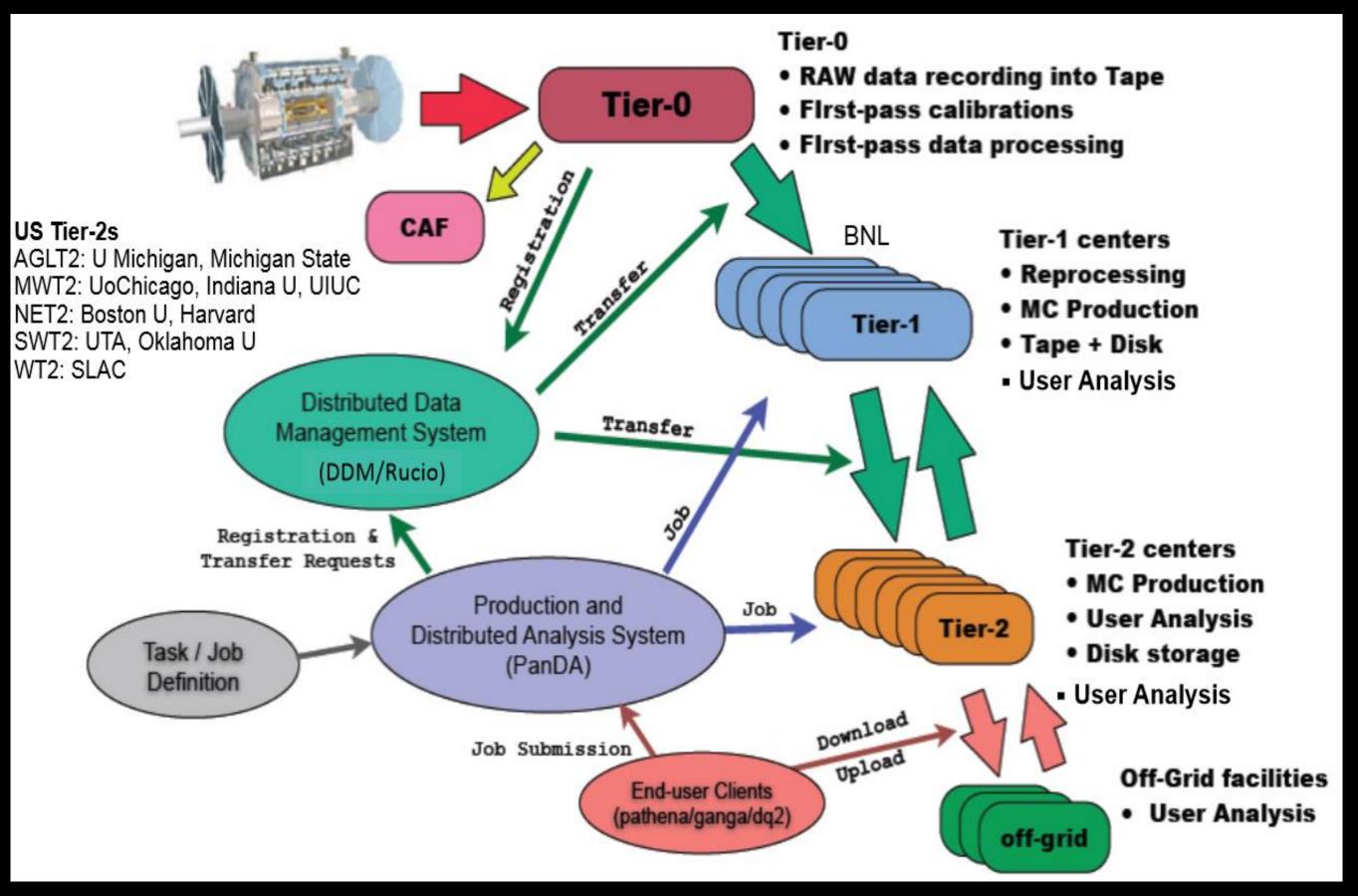
anywhere and everywhere



2010s: Uniform data access

Working towards transparent distributed data access enabled by the network and web

ATLAS Distributed Computing ...

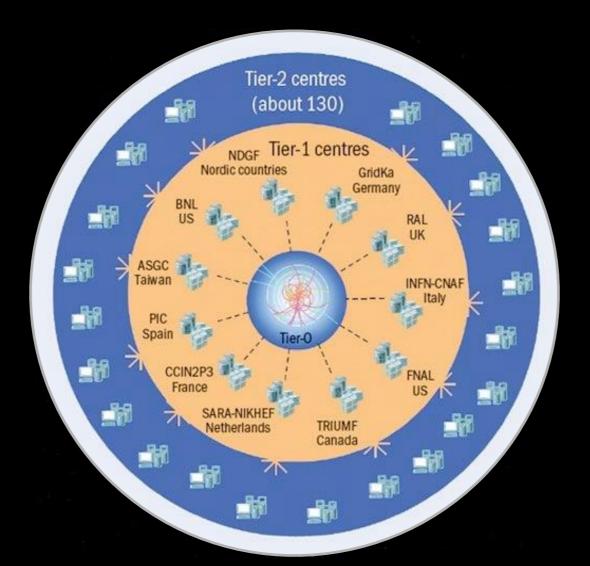


... Using a Global Computing Infrastructure

Tier-0 (CERN): data recording, reconstruction and distribution

Tier-1: permanent storage, re-processing, analysis

Tier-2: Simulation, end-user analysis



Nearly 160 sites in 35 countries

~350,000 cores

200 PB of storage

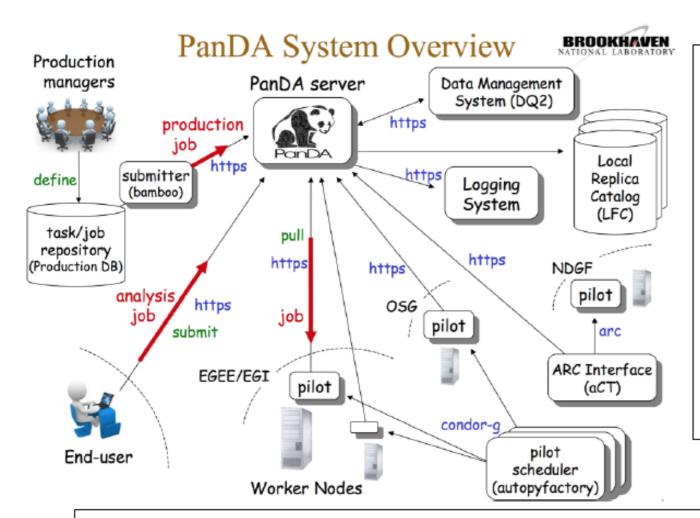
> 2 million jobs/day

10 and 100 Gb links

The Worldwide LHC Computing Grid

WLCG: An international collaboration to distribute and analyze LHC data. Integrates computer centers worldwide that provide computing and storage resources into a single infrastructure accessible by all LHC physicists

PanDA Workload Management System



BNL's Physics Applications Software (PAS) group leads development of the PanDA workload management system with UT Arlington PanDA manages processing and data workflows for large scale data intensive computing

- 2005: Initiated for US ATLAS
- 2008: Adopted ATLAS-wide
- 2009: First use beyond ATLAS
- 2012: ASCR/HEP funding for Exascale BigPanDA
- 2013-14: New PanDA based ATLAS prod system
- 2014: New Event Service fine grained processing
- 2014: PanDA community growing in HEP, NP, cosmology... US and international

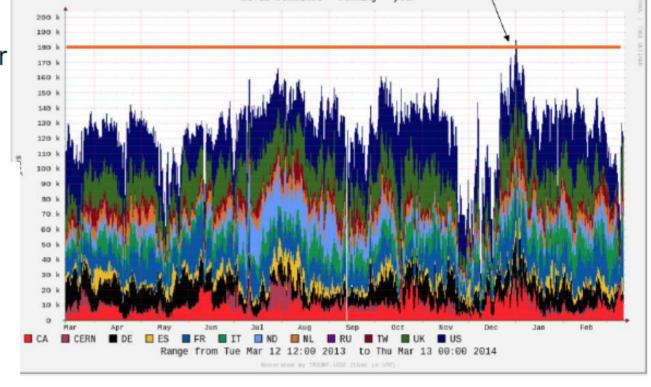
Global ATLAS PanDA operations:

Up to ~200k concurrent jobs, 1.5M/day, O(100M)/year ~1400 ATLAS users, ~140 sites

1.2 Exabytes per year processed (2013)

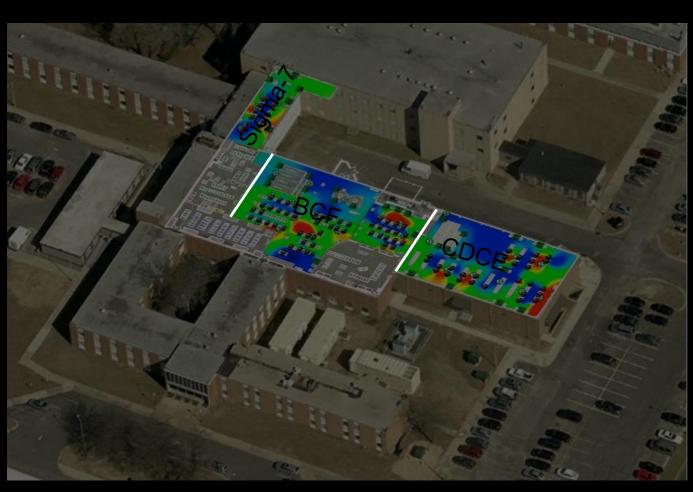
PAS also does software infrastructure, cloud & HPC porting, offline software development, leveraging new processor technologies, software project management... for BNL's HEP programs in all Frontiers, and the wider community

~ 180 k running jobs at peak



RACF at BNL: An Overview

 Formed in the mid-1990's to provide centralized computing resources for the four RHIC experiments (BRAHMS, PHOBOS, STAR, PHENIX)



- Role was expanded in the late 1990's to act as the US Tier-1 computing center for the ATLAS experiment at the LHC
- Small but growing neutrino and astrophysics presence (Daya Bay, LBNE, LSST)
- Located in the Brookhaven Computing Facility
- 30 FTEs providing a full range of scientific computing services for more than 4000 users

RACF: Setting The Scale

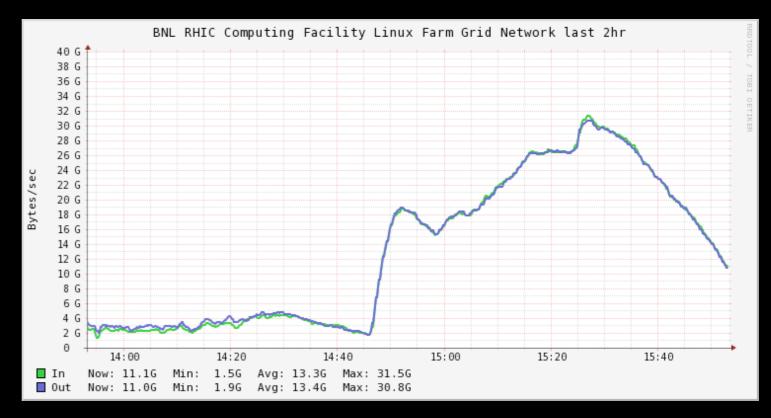
☐ RHIC

- 1300 COTS Compute Servers (32k logical CPU cores)
- 16 PB of Distributed Disk Storage on Compute Nodes, >1500
 Gb/s aggregate data transfer rates observed between servers

5 Robotic Tape Libraries w/ 50+ tape drives and 50k cartridge

slots





RACF: Setting The Scale

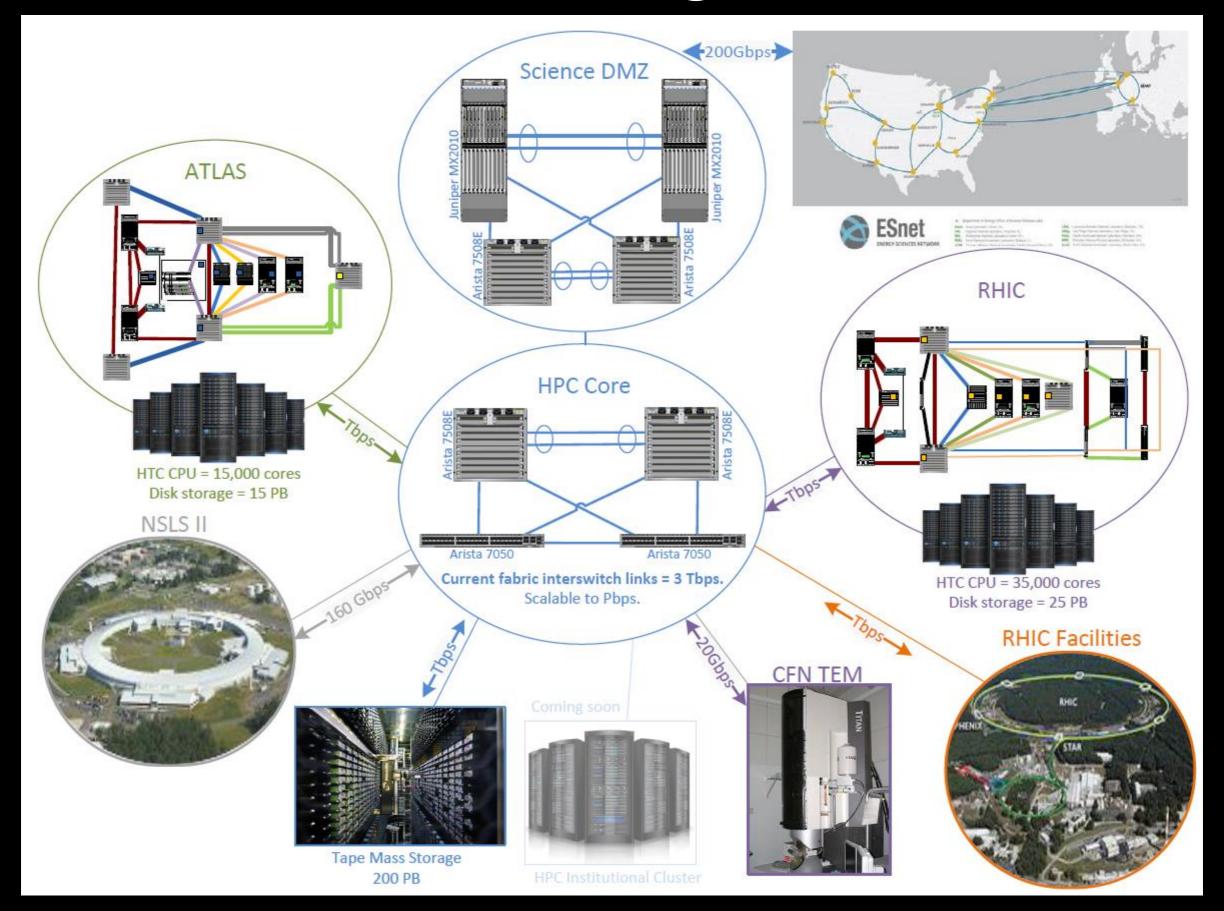
☐ ATLAS

- 830 COTS Compute Servers (17,000 CPU cores)
- 42 Dedicated Servers providing 13.6 PB of Disk Storage
- 4 Robotic Tape Libraries w/ 40 tape drives and 36k cartridge slots
- Magnetic Tape Archive (200 PB Capacity)
 - Data inventory of 60 PB on 58,000 tapes



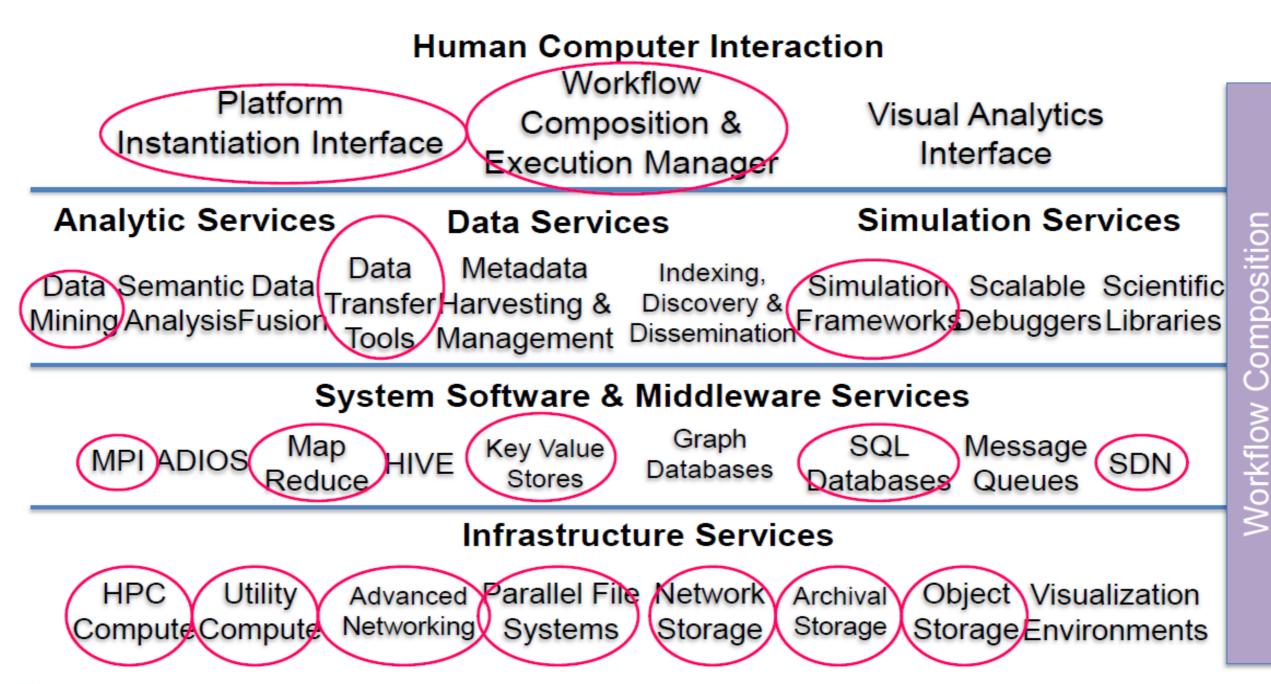


RACF — Setting the Scale



Our Infrastructure is Services

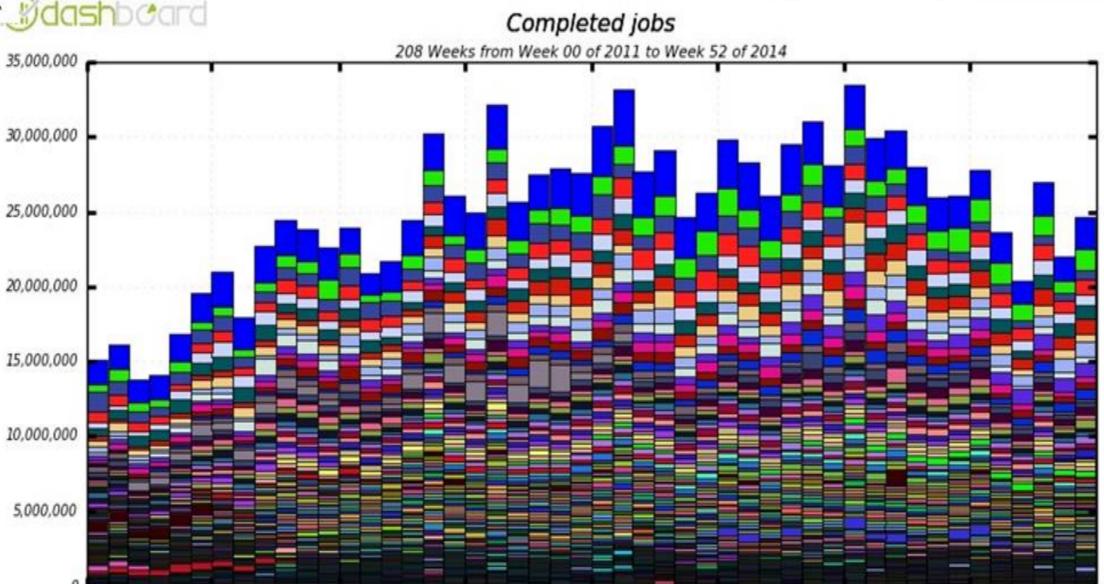
A rich environment of common services that can be flexibly composed to meet specific requirements of science domains across BNL and DOE SC





PanDA

ATLAS Workload – Managed by PanDA



lan 2013

Jul 2013

Global ATLAS PanDA operations

Jul 2011

lan 2012

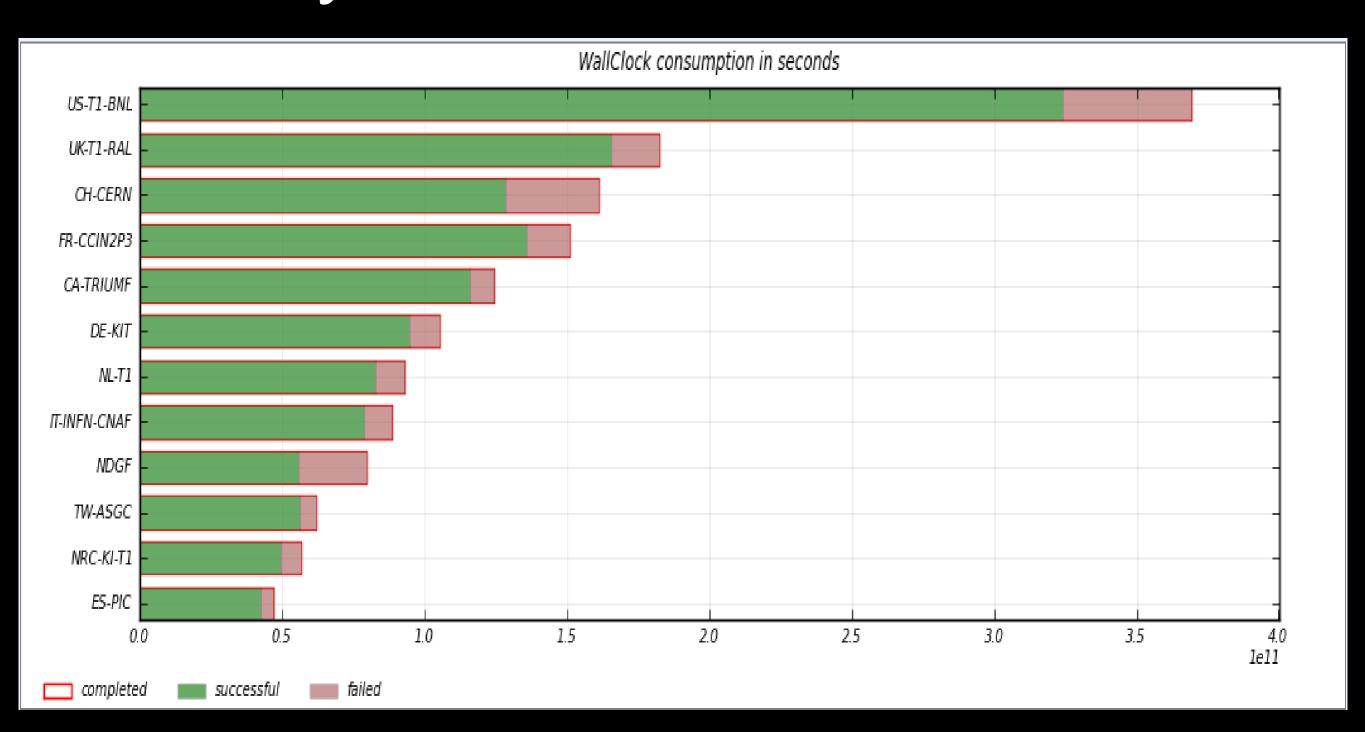
kıl 2012

Up to ~200k concurrent jobs 25-30M jobs/month at >100 sites ~1400 ATLAS users, ~140 sites 1.2 Exabytes processed in 2013
1.1 Exabytes in 2014
Exascale scientific data processing today

Jan 2014

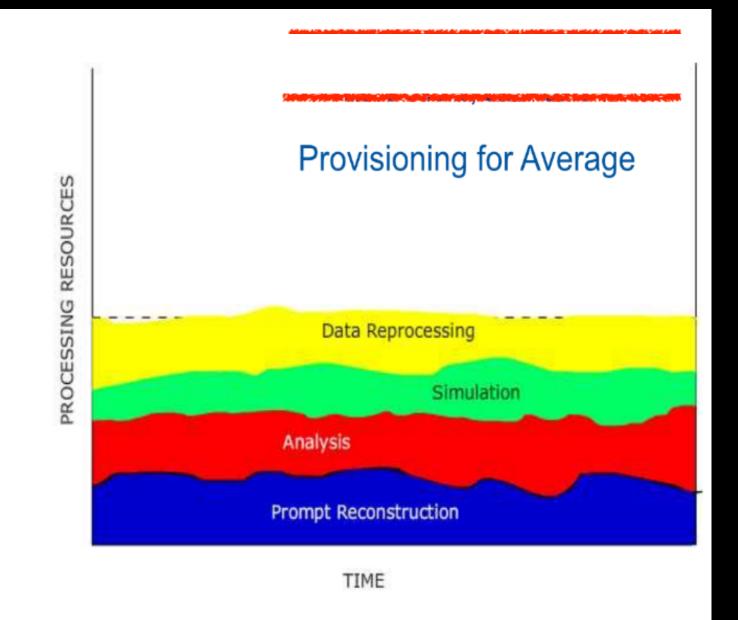
Jul 2014

ATLAS Processing Contribution by Tier-1 Site in 2015



Provisioning for Peak Demands

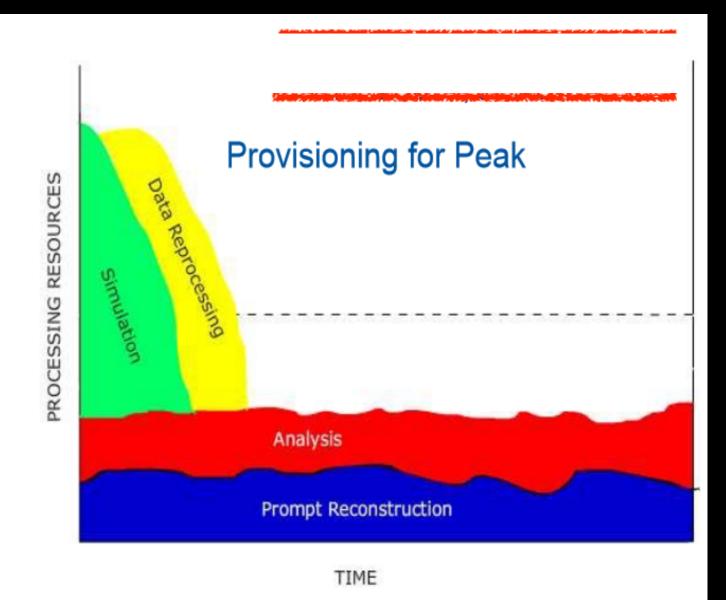
- The "dream" of short turn-around times for workflows
 - Short latencies in particular in analysis workflows are important for science efficiency
 - Use resources from a larger pool when they are needed, should also result in more cost-effective solutions
- Separating the processing and storage services allows them to scale independently
- e.g. ATLAS and CMS are looking at ways to double available resources for periods of time
 - using Amazon services



Provisioning for peak requires that we use pooled resource —> Clouds or large HPC Center!

Provisioning for Peak Demands

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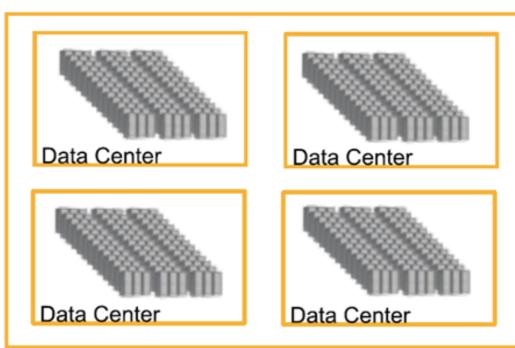


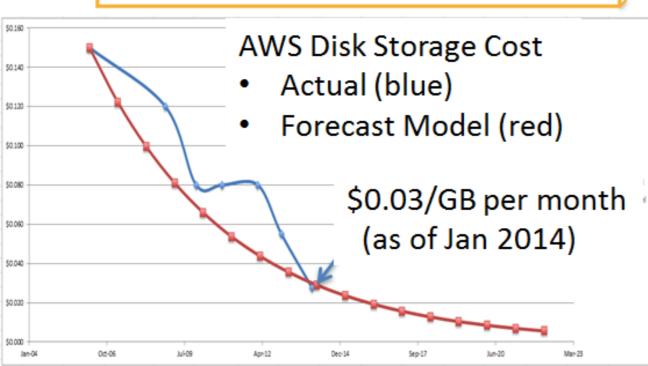
Provisioning for peak requires that we use pooled resource —> Clouds or large HPC Center!

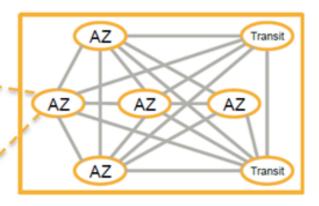
The Potential of Commercial Cloud Resources

A Snapshot of AWS Global Capacity

J. Kinney (AWS)







- 53 AWS Edge Locations
- 11 Regions
- 28 Availability Zones
- 2 or more AZs per Region
- 1-6 Data Centers per AZ
- 50,000-80,000+ servers per DC
- Up to 102 Tbps provisioned to each DC

Cost for Compute (AWS Spot) quickly approaching cost for dedicated resources

A cost-efficient way to serve peak demand

Running ATLAS Jobs in the Cloud – At Scale and at Low Cost

Joint Project (Amazon AWS, BNL/ATLAS, ESnet) to investigate feasibility (technically and financially) of large-scale usage of commercial cloud resources

- AWS: Provide expertise and guidance to BNL/ATLAS, credits for AWS service investigation and scale-out tests
- BNL: Provide ATLAS-compatible VM image and provisioning infrastructure, incl. demand-driven (i.e. via PanDA server API) VM lifecycle management (create, retire, terminate)
- ESnet: Provide high-performance (up to 100G) network connectivity between AWS facilities and sites connected to R&E networks (general peering and AWS Direct Connect)
- Has made AWS partially waive Egress traffic fee (at level of 15% of total bill)

Cost of AWS/EC2 spot slightly lower than dedicated farm resources at BNL

Running ATLAS Jobs in the Cloud – Experience

"Unlimited" spot resources available on demand

Had no issues ramping up quickly from 1000 to ~6000 8-core instances (several instance types) in a single (out of 3) AWS region in the U.S.

Ran at level of 6000 instances for a few days with very low fluctuation (VM instance termination) due to spot overbidding

<1% of total running VM instances were terminated by AWS while production jobs were running during a multi-day period

Most of the terminations occurred within the first hour after VM instance creation -> no cost to us

Public cloud dvantages: "Unlimited" horizontal scaling in AWS EC2/S3 in terms of network bandwidth between compute and storage. Very high performance Object Store at low cost (when used as temporary storage for intermediate data products)

Running ATLAS Jobs in the Cloud – Potential going forward

Combination of "unlimited" capacity whenever we need it and competitive pricing makes AWS (and presumably other commercial cloud providers) an ideal resource to cover peak demands

Could think of deploying only components (kind and quantities) & services at our dedicated data centers where cloud providers cannot cope (yet, i.e. technical capabilities and cost)

Potential to vastly reduce size and scope of our dedicated (and aging) hardware deployment

Potential to lower computing facility operations cost at improved performance (whenever the collaboration is in desperate need) and availability (e.g. the availability of AWS services is much higher than what WLCG sites provide)

Potential to vastly increase our flexibility

Using cloud computing makes us nimble whenever we need specific resources/platforms – temporarily or for long periods.

Running ATLAS Jobs in the Cloud – Matching Workloads

But all these wonderful things are not compatible with and/or applicable to our current processing model

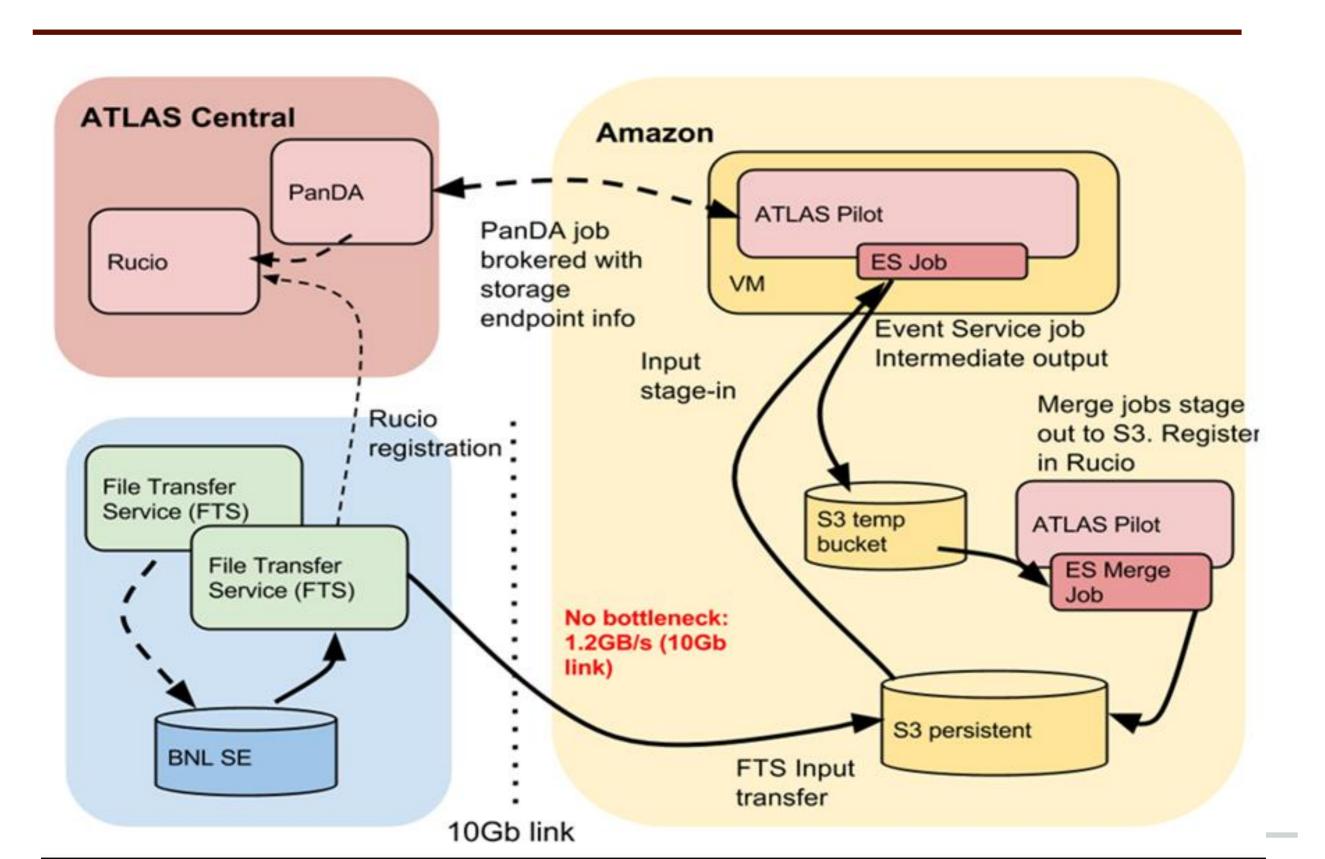
Most of our compute-intensive jobs run for 6-24 hours making spot VM instance terminations likely at probability of up to 80%

Potentially a huge waste of resources we would have to pay for

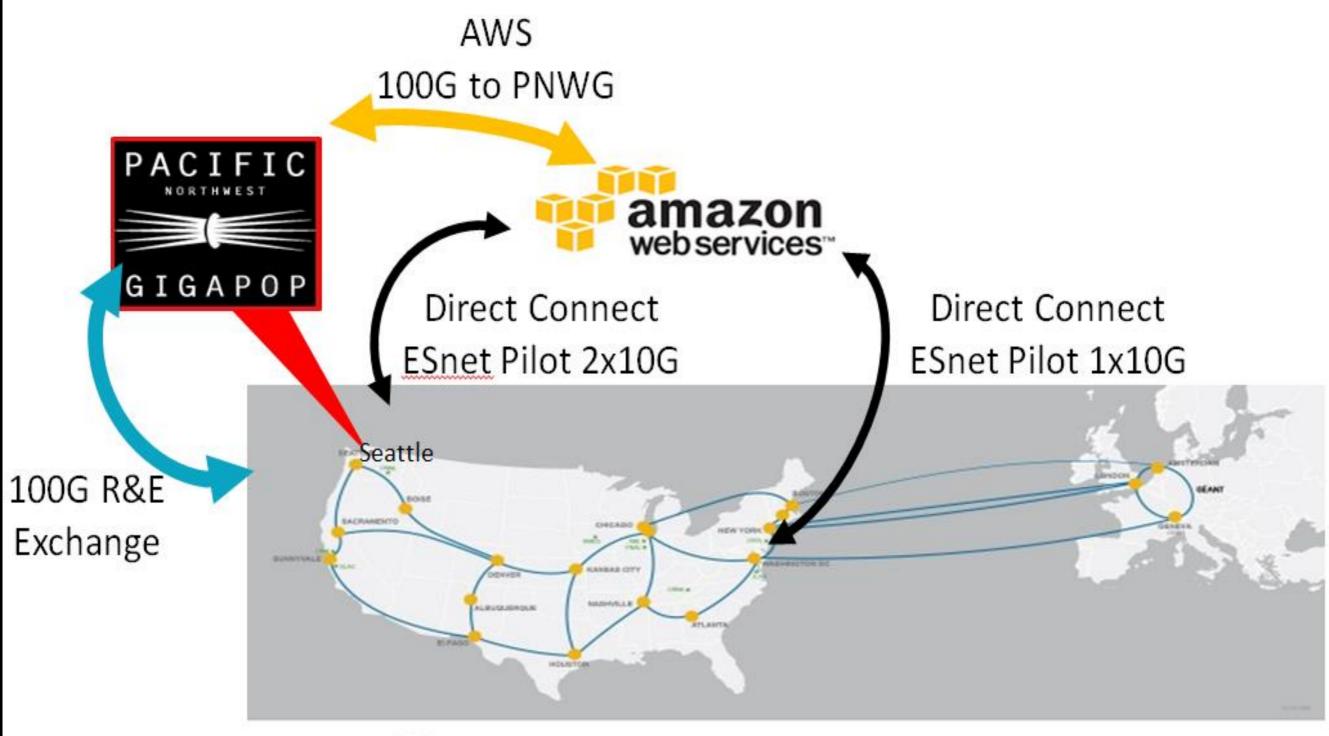
In a previous run we've observed 10-20% VM terminations (out of 2500 VM instances) with 2-hour jobs -> the shorter the job the better

- > ATLAS needs to match volatile and opportunistic resources with workload profile that suits the characteristics of a volatile resource
- Minimize loss due to resource becoming unavailable at any point in time
- The Event Server comes with all features that perfectly fit the characteristics of the AWS spot market
 - Fine-grained processing at the event level if we lose a VM we lose no more than a single event
 - Supports parallel processing at high degree can "grab" and utilize as many CPU resources as the provider can offer
 - Utilizes high performance Object Store technology this is the storage technology cloud providers have been focusing on

Event Server based Physics Event Simulation on AWS



Connecting AWS Facilities to the Research Community





Dispertment of Greegy Office of Science National Lide
 Amer. Areas Laboratory (Areas, IA)

ARRE Arrest Laboratory (Arrest A)

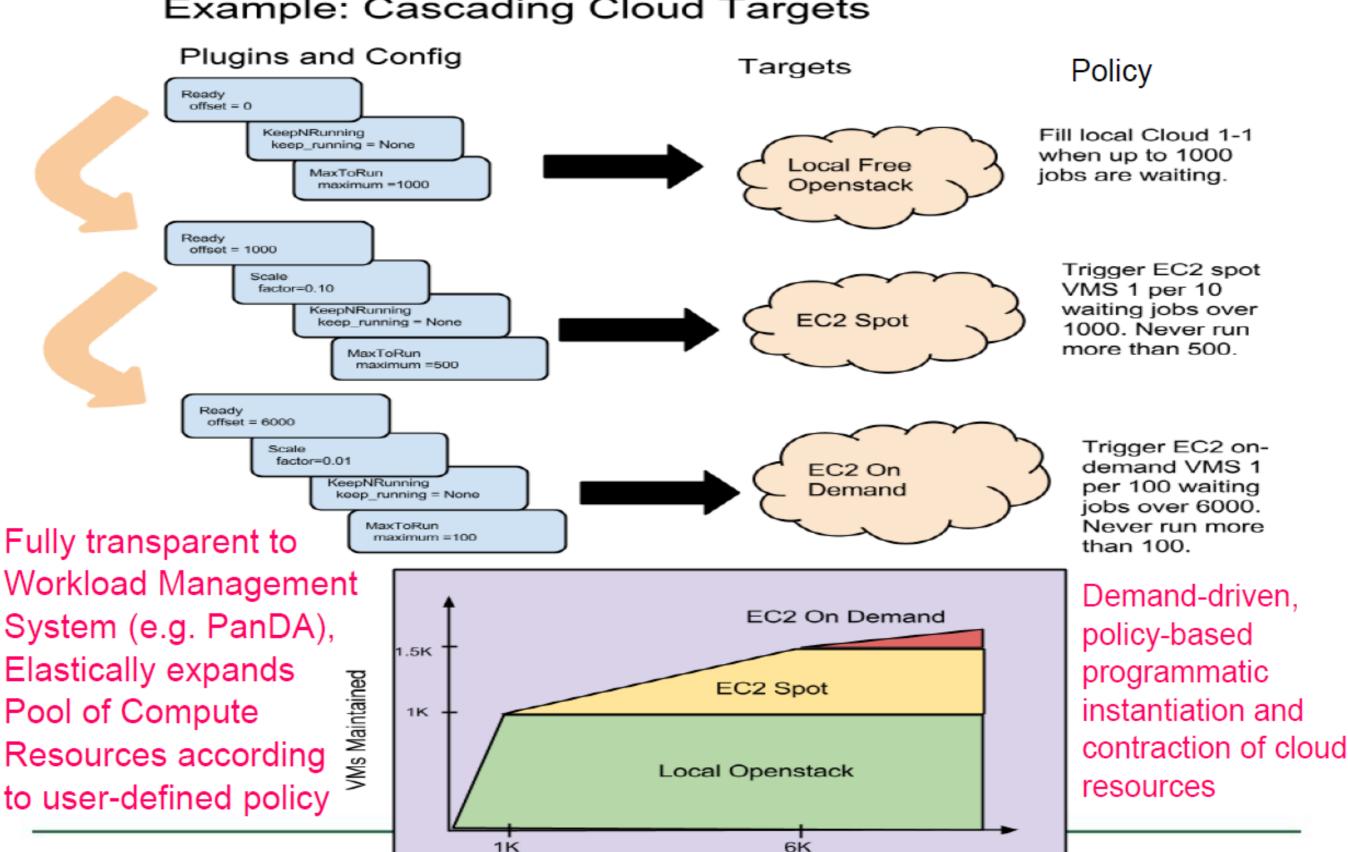
ARE Argumes National (alteratory (Argumes, X))

ESE, Drookhause National (alteratory (A)thon, NY)

(III) DRM, Cult Militar Catherine (atherine III)
PASE, Pacific Services Educated (atherine III)
PASE, Pricedin Plantin Physics (III)
Passiti, Pascont Service (III)
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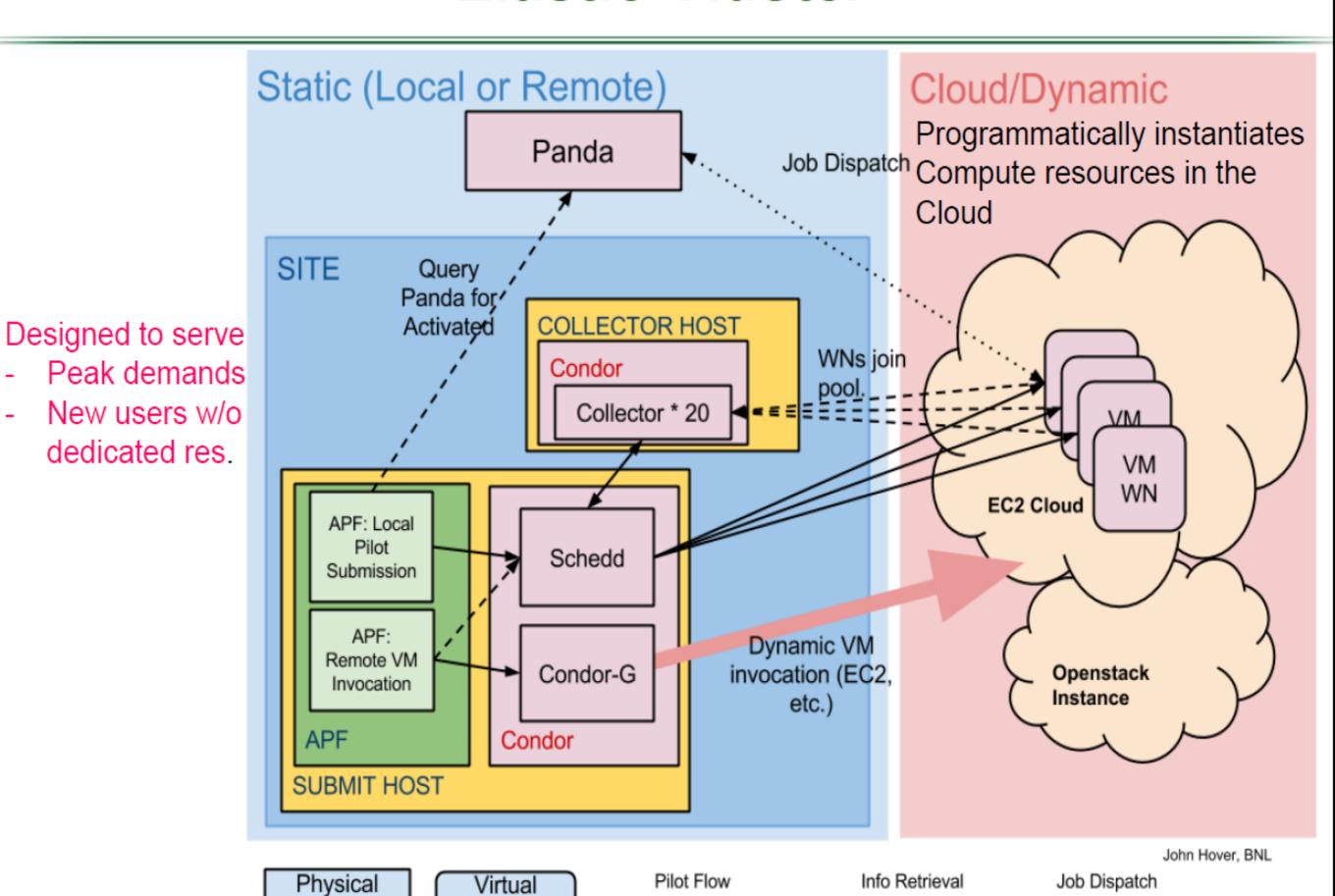
Using Cloud Resources effectively: A Policy-based Cloud Scheduler, developed at RACF

Example: Cascading Cloud Targets



Number Waiting

Elastic Cluster



Virtual

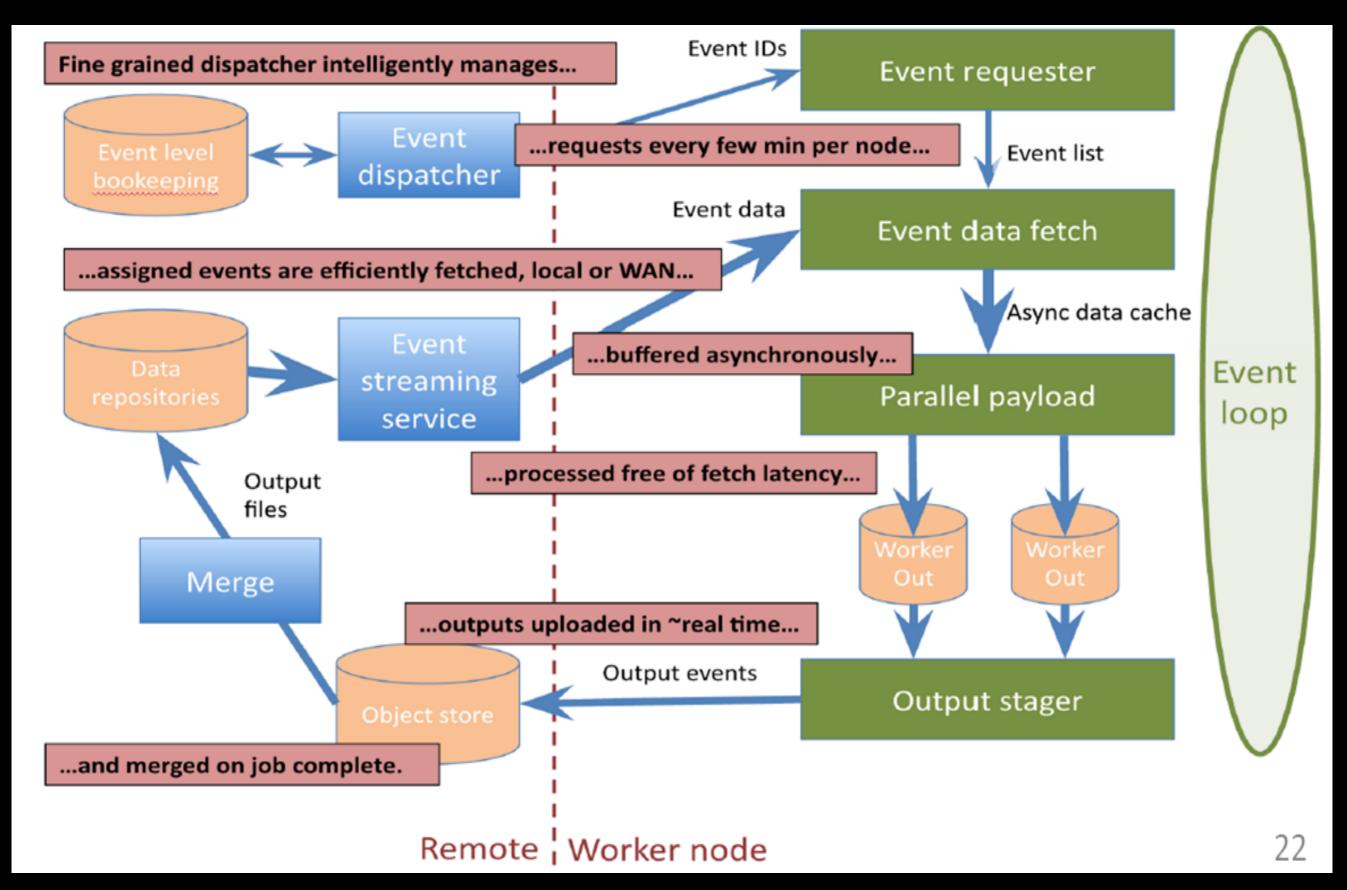
Host

host

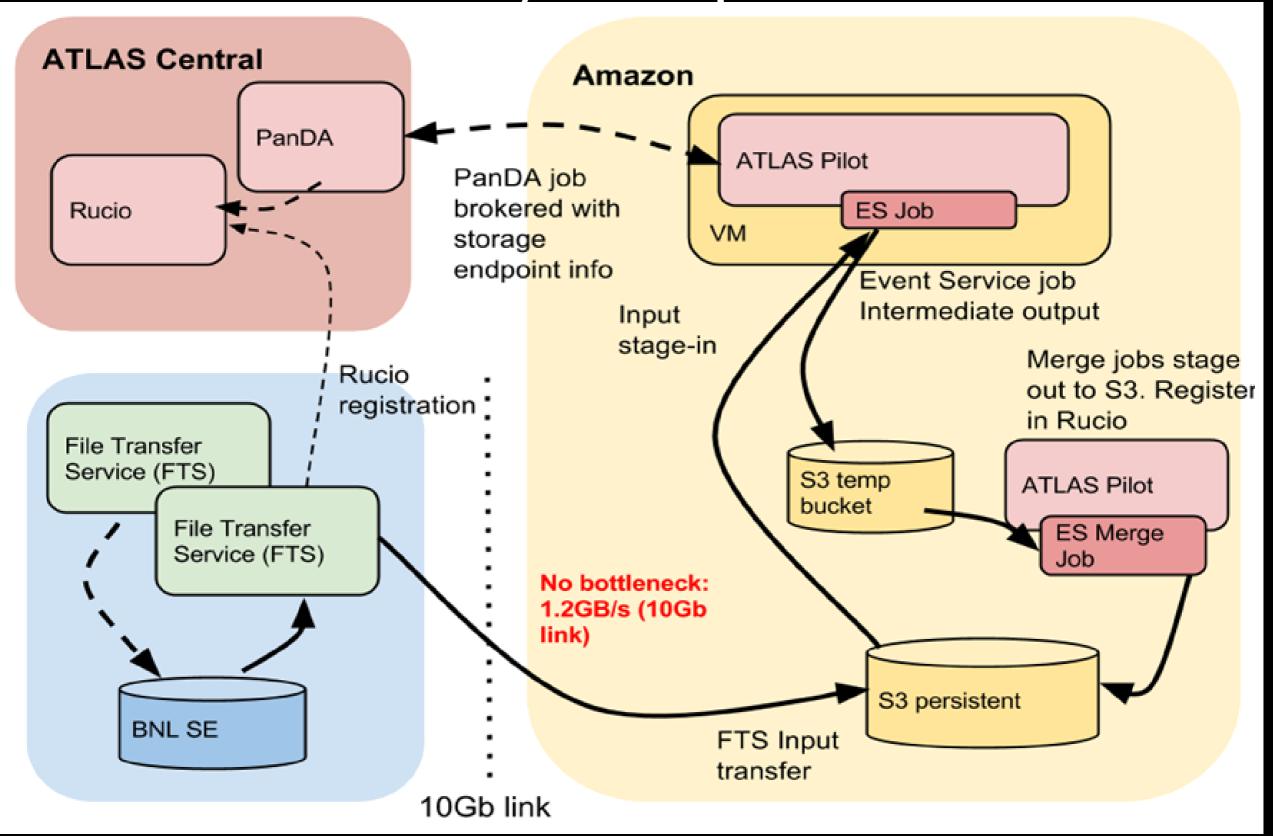
ATLAS Event Processing

- ATHENA ATLAS simulation, reconstruction and data analysis
 - Huge Codebase: millions of lines of code organized into thousands of independent software packages
 - Designed and developed over many years for sequential processing only
 - Static workload
 - Job processes a predefined sequence of events from a given file
 - Only after processing all events from the statically allocated workload the job is considered
 - In case of premature termination the job is considered failed and all data produced by the job is lost

The ATLAS Event Service

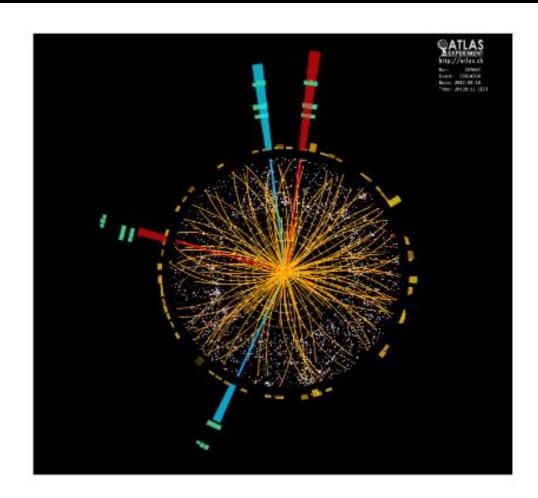


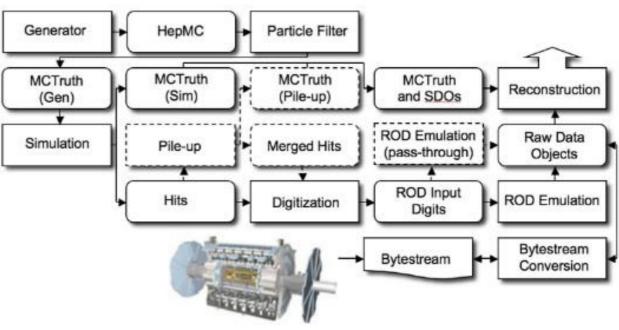
Architectural Overview from the Facility Perspective



Simulation is important and resource intensive

- We collide particles together and measure the trajectories of the products in our detectors
- We then compare these results with simulation – at multiple levels
 - Does the detector respond to these particles in the way we expect?
 - Do we see the number of particles in various categories that we expect?
 - Etc.
- This is a complex process, and we are as dependent on the simulation chain as we are on the data chain.
 - ATLAS uses about a billion cpu-hours per year on this.





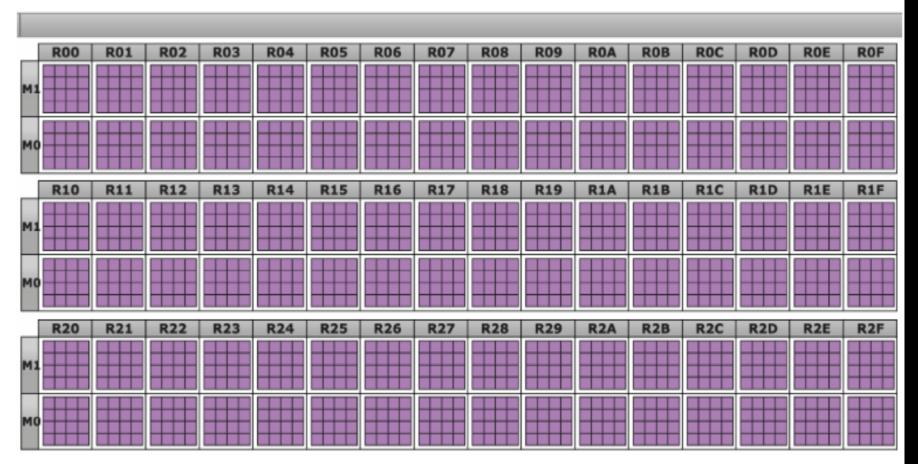
Computing to reach the Science Goals

- ATLAS uses about a billion CPU-hours per year on the Grid
 - This does not include the cycles spent calibrating or reconstructing the data; the problem is defined as what happens after this point
- Event Generation
 - Simulate the physics process of interest: produces lists of particles and their momenta
- Simulation
 - Simulate the interaction of these particles with the detector
 - You may have heard the term "Geant" or "G4". Geant4
 is the toolkit by which we do this.
- Reconstruction and Analysis
 - Treat the simulated data as real, reconstruct the particles, and do the final analysis

The Power of a Supercomputer

- We can run using the entire machine
 - For throughput reasons, we normally limit ourselves to 1/3 of the machine: a million parallel processes
- Per core event generation rate is ~1.5x a Grid core
 - Speedup of x23 over the year
 - Mira has a lot of cores! (768432)

Computing Facility Mira Activity



While this job was running, Mira was producing the equivalent computing as 5 or 6 ATLAS Grids.

On our best days, we provide the equivalent computing capacity of the whole ATLAS Grid.







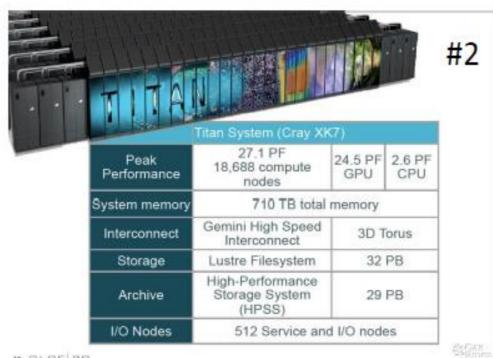




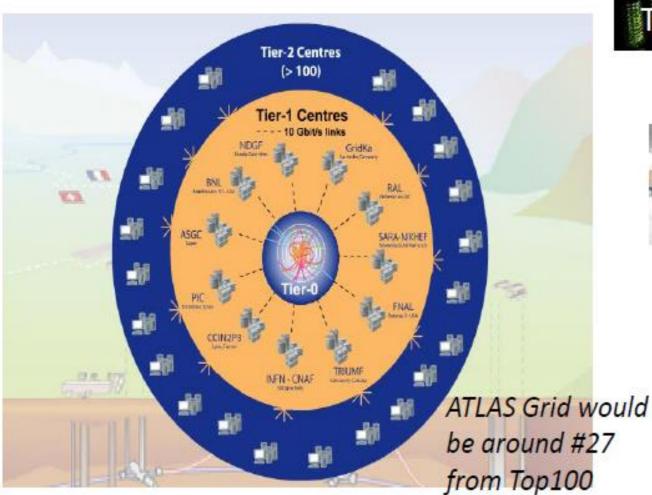














#7

The ATLAS collaboration have members with access to these machines and to many others...

ASCR Computing Upgrades

System attributes	NERSC	OLCF	ALCF	NERSC Upgrade	OLCF Upgrade	ALCF Upgrades	
System attributes	Now	Now	Now	NERSC Opgrade	OLCF Opgrade		
Name Planned Installation	Edison	TITAN	MIRA	Cori 2016	Summit 2017-2018	Theta 2016	Aurora 2018-2019
System peak (PF)	2.6	27	10	> 30	150 -> 200	>8.5	180
Peak Power (MW)	2	9	4.8	< 3.7	10	1.7	13
Total system memory	357 TB	710TB	768TB	~1 PB DDR4 + High Bandwidth Memory (HBM)+1.5PB persistent memory	> 1.74 PB DDR4 + HBM + 2.8 PB persistent memory	>480 TB DDR4 + High Bandwidth Memory (HBM)	> 7 PB High Bandwidth On- Package Memory Local Memory and Persistent Memory
Node performance (TF)	0.460	1.452	0.204	> 3	> 40	> 3	> 17 times Mira
Node processors	Intel Ivy Bridge	AMD Opteron Nvidia Kepler	64-bit PowerPC A2	Intel Knights Landing many core CPUs Intel Haswell CPU in data partition	Multiple IBM Power9 CPUs & multiple Nvidia Voltas GPUS	Intel Knights Landing Xeon Phi many core CPUs	Knights Hill Xeon Phi many core CPUs
System size (nodes)	5,600 nodes	18,688 nodes	49,152	9,300 nodes 1,900 nodes in data partition	~3,500 nodes	>2,500 nodes	>50,000 nodes
System Interconnect	Aries	Gemini	5D Torus	Aries	Dual Rail EDR- IB	Aries	2 nd Generation Intel Omni-Path Architecture
File System	7.6 PB 168 GB/s, Lustre [®]	32 PB 1 TB/s, Lustre [®]	26 PB 300 GB/s GPFS™	28 PB 744 GB/s Lustre [®]	120 PB 1 TB/s GPFS™	10PB, 210 GB/s Lustre initial	150 PB 1 TB/s Lustre [®]

Phase Space of available & affordable Resources

10,000 feet overview

Grid

- Virtual
 Organizations
 (VOs) of users
 trusted by Grid sites
- VOs get allocations
 - → Pledges
 - Unused allocations: opportunistic resources

Trust Federation

Cloud

- Community Clouds -Similar trust federation to Grids
- Commercial Clouds Pay-As-You-Go model
 - Strongly accounted
 - Near-infinite capacity →
 Elasticity
 - Spot price market

Economic Model

HPC

- Researchers granted access to HPC installations
- Peer review committees award

Allocations

 Awards model designed for individual PIs rather than large collaborations

Grant Allocation

This new paradigm significantly changes the role of Facilities in providing end-to-end solutions to their customers

- Facilities can benefit from providing a much more "elastic" offering
- Moving away from stand-alone stove-piped facilities toward Labs providing leadership role in the computing eco-system
 - labs, leadership class and production class facilities, etc are part of and leaders in the eco system, that includes scientific and commercial providers
 - sites will find a large "market" for specific offerings: specialized architectures, archival capabilities, database services, data management solutions
 - the eco-system is enabled by the labs and OSG and others
- Facility's role is still to provide "complete solutions" for their users
 - CPU and data capacities with guaranteed level of service
 - Users would not have to care about wether their jobs are running on "owned" or "rented" resources Sites could make the economic decision themselves and optimize their cost structure
 - Storage services that adapt to where the jobs are running
 - On-demand services that scale by tapping into large pooled resources
 - like clouds, HPC, OSG etc

Trends across the HPC Landscape

- Increasing importance of computing and simulation within SC and DOE programs (across our missions: science, national security, and quest for cleaner energy)
 - Continued full subscription of computational resources
 - Increasing importance of effective partnerships (domain + applied math + CS)
 - Difficulties persist in acquiring and retaining highly skilled workforce
- Nexus of big data and powerful compute is an emerging frontier
- The drive toward exascale Scientifically important and challenging questions await exascale
 - Dennard scaling is driving further increases in concurrency → billion-way concurrency is coming
 - Post-CORAL computer architectures may be significantly different → significant recoding
 - Data movement is increasingly costly → becoming the rate limiter
 - Power consumption remains an issue (\$1M/megawatt-year)
 - A petaflop in a 19-inch rack

S. Binkley/ ASCR

The post-Moore's Law epoch is drawing nearer – we need to start preparing

Post Moore's Law Computing

- CMOS lithographic feature sizes are approaching fundamental limits
 - Currently at 22 nm (both Intel and Nvidia)
 - 11 nm is projected for ~2015 2016 (both Intel and Nvidia)
 - However, gate lengths may be smaller than 6 nm corresponding gate dielectric thickness may reach a monolayer or less
 - The industry roadmap reaches beyond 11 nm (7 nm and 5 nm) but may be unattainable
 - Non-silicon extensions of CMOS, e.g., using III-V materials or nanotubes/nanowires or non-CMOS technoligies, including molecular electronics, spin-based computing, single-electron devices, and graphene have been proposed
 - At scales of ~10 nm, quantum tunneling may become significant
 - Capital costs for tooling are increasing dramatically as feature sizes shrink

Options:

- Computing using superconducting technologies
- Quantum computing/quantum information science
- Neuromorphic computing
- Probabilistic computing

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Considerable R&D required

S. Binkley/ASCR

Summary and Outlook

- There is no end in sight for large increases in resource demands and new capabilities, which change expectations and requirements on HEP facilities
 - provide services to distributed communities, supporting complex end-to-end use cases involving huge computational and data throughput needs and capabilities
- The role of the facility providers are changing as they are facing cost effective competition to their "bare metal" offerings from laaS providers
 - Facilities remain to be first-line support for the complex scientific work flows and data management needs of HEP and other DOE SC communities
 - Facilities should integrate new opportunities and capabilities into their service offerings, in particular in connecting to large data management and data access systems, beyond "login and batch" services for applications and application libraries
- Facilities should keep an open mind how to provide their services so they fit into and enrich the US and international scientific computing eco-system
 - requires new thinking and approaches to difficult issues in the distributed environment, including security, robustness and protection of resources, accounting, prioritization etc
 - good experiences with LHC and emerging IF experiments
- HEP and other DOE Facilities clearly have a huge opportunity for great leadership roles in this environment